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THEMATIC ISSUE

Hydraulic fracturing in unconventional gas reservoirs: risks in the geological system part 1

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Abstract Hydraulic fracturing of unconventional gas reservoirs rapidly developed especially in the USA to an industrial scale during the last decade. Potential adverse effects such as the deterioration of the quality of exploitable groundwater resources, areal footprints, or even the climate impact were not assessed. Because hydraulic fracturing has already been practised for a long time also in conventional reservoirs, the expansion into the unconventional domain was considered to be just a minor but not a technological step, with potential environmental risks. Thus, safety and environmental protection regulations were not critically developed or refined. Consequently, virtually no baseline conditions were documented before on-site applications as proof of evidence for the net effect of environmental impacts. Not only growing concerns in the general public, but also in the administrations in Germany promoted the commissioning of several expert opinions, evaluating safety, potential risks, and footprints of the technology in focus. The first two publications of the workgroup "Risks in the Geological System" of the independent "Information and Dialogue process on hydraulic fracturing" (commissioned by ExxonMobil Production Deutschland GmbH) comprises the strategy and approaches to identify and assess the potential risks of groundwater contamination of the exploitable groundwater system in the context of hydraulic fracturing operations in the Münsterland cretaceous basin and the Lower Saxony Basin, Germany. While being specific with respect to local geology and the estimation of effective hydraulic parameters, generalized concepts for the contamination risk assessment were developed. The work focuses on barrier effectiveness of different units of the overburden with respect to the migration of fracking fluids and methane, and considers fault zones as potential fluid pathway structures.

Keywords Hydraulic fracturing · Risk assessment · Fracking fluid · Methane · Barrier rocks

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Introduction

General

The dialogue and information dissemination process on hydraulic fracturing of unconventional gas reservoirs was commissioned by ExxonMobil Production Deutschland GmbH in 2011 as a first comprehensive approach to study possible impacts of the technology on man and the environment in Germany and was conducted by several interdisciplinary scientific working groups (Ewen et al. 2012). In this publication, the first part of the main results of the workgroup "Risks in the Geological System" is presented.

It will discuss the overall assessment approach, the definition of appropriate model scenarios for different time and space scales, methods to characterize the hydrogeological system, as well as the results and recommendations. The aim is to provide a basis for the assessment of the contamination risk of the shallow groundwater systems in the Lower Saxony Basin (LSB, southern extension of the North German Basin (NGB) and the Münsterland Cretaceous Basin (MCB)—i.e. geographically specific regions—following hydraulic fracturing operations in existing deep unconventional gas reservoirs. Despite the initial concentration of the work on geographically specific regions, the group is of the opinion that the conclusions arrived at can provide generally applicable information and systematics for the assessment of the contamination risks associated with fracking operations. The second paper presents the results of the workgroup concerning the simulation of the model. The transport of the fracking fluids is simulated using established mathematical modelling techniques. Input to the models are model geometry, hydraulic and transport parameters, as well as boundary conditions (cf. part 2, Kissinger et al. 2013). A simplified map presenting the site locations in the investigation areas of the MCB and the LSB is shown in Fig. 1.

Unconventional gas reservoirs

In unconventional reservoirs the natural gas is locked in compact low-permeability sedimentary units that has to be artificially fractured in order to provide the necessary porosity and permeability to enable commercial gas extraction. Two major types are distinguished. While in the MCB coal bed methane (CBM) is the principal gas resource, shale gas prevails in the LSB. So-called tight-gas reservoirs take up an intermediate position between unconventional and conventional reservoirs since not porosity but permeability is the limiting factor for gas migration. Resources at depths of more than 4,000 m north of the investigated sites in the LSB or NGB, respectively, were not considered.

Environmental risks related to the development of unconventional gas resources

The 'risks in the geological system' that are associated with hydraulic fracturing of deep unconventional reservoirs are manifold. They comprise contamination risks for the exploitable groundwater sources from the toxic components of the injected fracking fluids, from mobilized formation fluids, or methane escaping through fractures and faults, or due to problems in the technical system, i.e. leaks through the casing and borehole annulus. The latter is being investigated in the contribution of Uth (2012). Potential adverse effects for the environment caused by chemical compounds in present-day fracking fluids are directly related to their toxicity for organisms. For that reason human toxicities and ecotoxicities of the respective substances were evaluated in a comprehensive survey by two groups of experts within the dialogue process (Gordalla et al. 2013; Riedl et al. 2013). However, the mainly organogenic contaminants would be strongly affected in the subsoils by degradation and metabolic transformation. Other impacts on human or the environment often associated not only with unconventional, but also conventional or geothermal reservoir operations are earthquakes, groundwater contamination by remote re-injection of formation water (e.g. Olsson et al. 2013) or directly on the surface by accidents.

The current intensive public debates between the different stakeholders about the various potential risks are strongly affected by the complexity of the subject. Further, it is not only difficult for these interest groups, but also for professionals that might be new to the topic to differentiate between information that bases on facts, opinions or individual interpretations of what happens or what was measured. Thus, transparency and free access to fact based information are necessary to facilitate the public discussion process. Such platforms have been developed for example in Germany during the last years including the "The dialogue and information dissemination process on hydraulic fracturing" (Ewen et al. 2012) or the Web-based "Shale gas information platform (SHIP)" (Hübner et al. 2013).

Overall approach

Deterministic, conservative approach

In order to assess the risk of any activity, i.e. the likelihood of the occurrence of a defined adverse effect of fracking operations, either probabilistic or deterministic approaches can generally be chosen. The basis for the probabilistic approach is a comprehensive database, resulting from the monitoring of the effect of the respective activity (here the

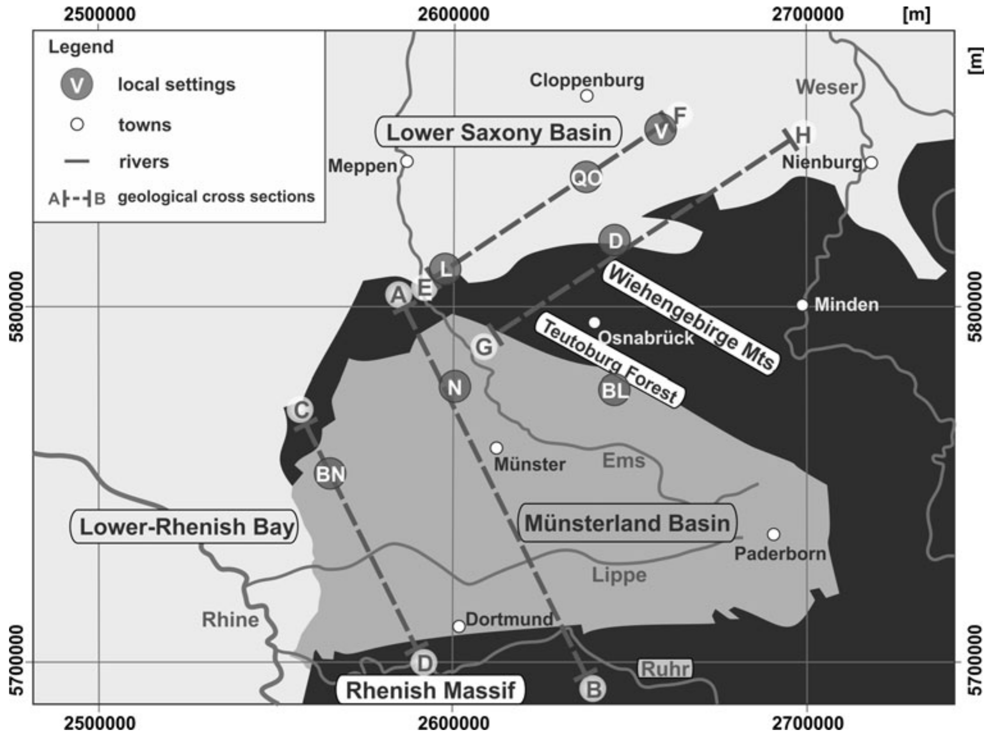

Fig. 1 Simplified map presenting the site locations in the investigated area of the Münsterland Cretaceous Basins and the Lower Saxony Basin, northern Germany. The site locations are indicated with *letters*: *BN* Borken-Nord, *N* Nordwalde, *BL* Bad Laer, *L* Lünne, *D* Damme, *QO* Quakenbrück-Ortland, *V* Vechta)

spreading of the fracking fluids in the subsurface). This requires that the actual monitoring process be designed so that potentially uncontrolled spreading can be detected. The above probabilistic approach has the advantage that the database covers a large spectrum of operational conditions as well as the natural variability of geological and hydrogeological situations and parameters. The deterministic approach, i.e. physics-based, has the advantage of being transparent and with high predictive power once the system and processes are understood and the system geometry and parameters are available. The latter two ingredients, however, require comprehensive characterization efforts, which, in the field of the fluid spreading during the fracking process, are not available yet.

Here, the deterministic approach was chosen, because a database for a serious probabilistic analysis does not yet exist. To compensate data gaps of the actual hydraulic parameters at the investigated locations, the strategy selected to estimate the spreading of the fracking fluids and methane, was based on a pronounced conservative approach. That implies the assumption that several unfavourable factors accumulate thus providing limits beyond which contaminant transport would be highly implausible. The unfavourable factors considered here are related to (a) contaminant migration processes (only advection, processes slowing down contaminant spreading, such as matrix diffusion, adsorption, degradation/metabolic transformation are not being considered); (b) system geometry (entry of the fracking fluids directly at the base of the permeable groundwater system channelled via a fault zone); (c) system parameters (still plausible, but highest permeabilities and lowest effective porosities for overburden rocks and fault zones); and (d) boundary conditions (cf. Kissinger et al. 2013).

In sum, the results to be expected from the simulation process, although physically possible, are highly unlikely to be observed in nature, but they assist, together with a sensitivity analysis, in assessing the bandwidth of the extent of fluid migration and therefore help to realistically assess an upper margin of the risk, emanating from the subsurface fluid transport processes. Implausible combinations, such as high hydraulic conductivities paired with very low effective porosities were excluded. Implausible combinations, such as high permeabilities paired with very low effective porosities were excluded from the set of overburden properties. However, along faults, the combination of higher permeabilities and lower porosities apply and were accounted for to simulate flow and transport conditions.

The process of hydraulic fracturing and fracture generation

An important question to answer was the model representation of the target horizons. Since the natural system is highly heterogeneous with respect to the geomechanical parameters and highly variable with respect to the stress distribution, large variability regarding frac dimensions can be expected for variable operational conditions. A thorough study that includes the simulation of related processes would therefore require enormous effort. During the investigation process, information on the geometry of the individual fractures from microseismic and tiltmeter monitoring data became available through the Pinnacle-Halliburton study (Fisher and Warpinski 2011). Thousands of individual fracture treatments were investigated as to their vertical extent above the casing perforation level. Figure 2 illustrates the relation between depth of the fracking operation and vertical extents of the fracs.

The fracture treatments covered a wide spectrum of operating and geological parameters and therefore the measured data are believed to comprise potentially occurring conditions during fracture generation and are therefore considered as representative as a boundary condition to the model. Furthermore, the data suggest that the maximum vertical extent of the fractures is ca. 500 m (ca. 1,500 ft) above the casing perforation level. Concerns exist that uncontrolled fracturing might extend right into the shallow aquifers. The actual field data provide extremely valuable information for fracture dimensions under natural geological situations for generally applied operating conditions and demonstrate that these concerns are unfounded.

The authors plausibly and mechanistically explain the well-documented data set, derived from microseismic tiltmeter measurements in a comprehensive study. Maximum vertical extent of the fractures is ca. 500 m (1,500 ft), usually associated with existing fault zones and the vertical frac dimension decreases with decreasing thickness of the overburden.

The main finding of this important study is that the vertical fracture growth is limited as a result of a number of reasons, such as self-limitation effects (higher fluid pressures due to increased friction in complex fracture networks rather open up in a horizontal than vertical direction), impairing effects (vertical growth decreases at the cost of widening due to variations in vertical stress), mechanical refraction effects (due to layered structure of sediment deposits), leak-off effects (loss of fluid pressure into zones of higher permeability such as sandstones or intruded fault structures), and depth effects (vertical changes of the stress-fluid pressure difference cause pronounced widening at the upper tip of the frac at the cost of the available injection volume).

Based on the above, the group decided to divide the lower model boundary into a no-flow boundary for the major part and a constant pressure or constant flux [>0 (L^3 T^{-1})] boundary (depending on the simulated process) for a small area that represents a direct connection to a hydraulic fracture. The latter is assumed to be created during the hydraulic fracturing operation and thus connects the lower model boundary with the actual target layer below that is not part of the simulation domain (cf. Kissinger et al. 2013).

Identification of main system components, pathways, and scales

After determining the overall approach to be deterministic or physics-based and the representation of the hydraulic fractures and the target horizon in terms of boundary conditions, the modelling strategies depend on the local hydrogeological conditions and the conservative approach already defined and explained above.

However, two further factors of major importance in the risk assessment process are the scales of time and space that are needed to be considered. The lifetime of a specific

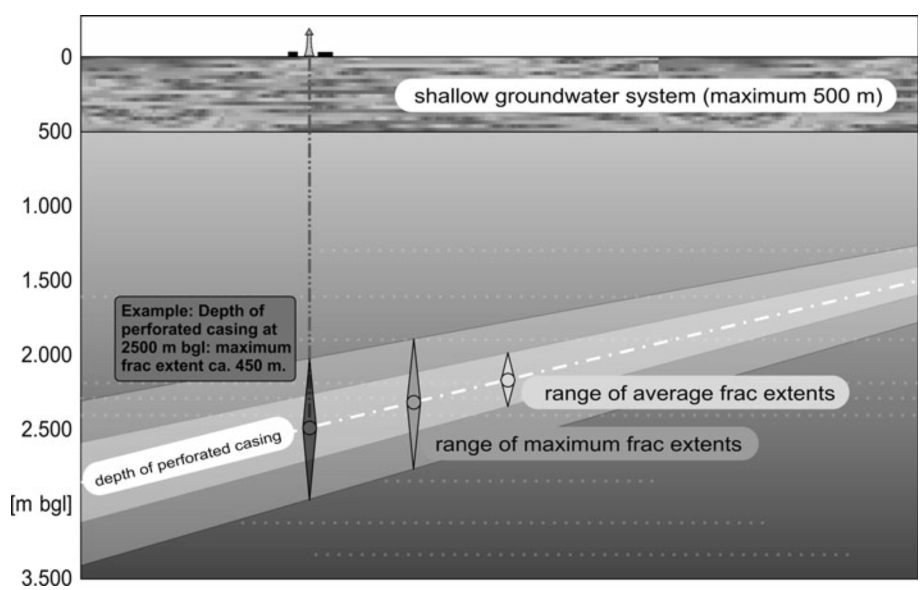

Fig. 2 Generalized diagram depicting the dependence of the average and maximum vertical extents of hydraulic fractures on depths between 2,800 and 1,500 m bgl measured at various sites in the Barnett-Shale, USA (after Fisher and Warpinski 2011)

site can be split up into three stages: (1) the development phase where hydraulic fracturing operations prepare the reservoir for production; (2) the production phase and (3) the post-production phase. However, reservoir enhancement during the production phase by additional hydraulic fracturing applications is often necessary. Figure 3 illustrates the general setup of the system analysed in this study.

The hydraulic fracturing operations usually last for about 12 h. While the maximum pressure is kept for about 2 h, the remaining time accounts for the passive pressure decline. During this short time period, the injected fluid is allowed to migrate upward on a local scale due to the imposed high-pressure gradient. The procedure directly after the high-pressure phase depends on the applied fracturing and breaker fluid systems. Any fracking fluid that escaped from the target formation would be exposed to regional and long-term migration if a hydraulic gradient exists. To allow the methane gas to migrate into the fracture system and to the well the hydraulic gradient is directed to the well throughout the production phase. In the post-production phase when the pressure gradient to the production well is terminated methane that remained in the reservoir eventually could be allowed to migrate upward for an even longer period based on gravitational forces depending on the prevailing properties of the overburden. Thus, the modelling strategy and the scenarios developed have to be adapted to the different stages of a site with different spatial and temporal scales.

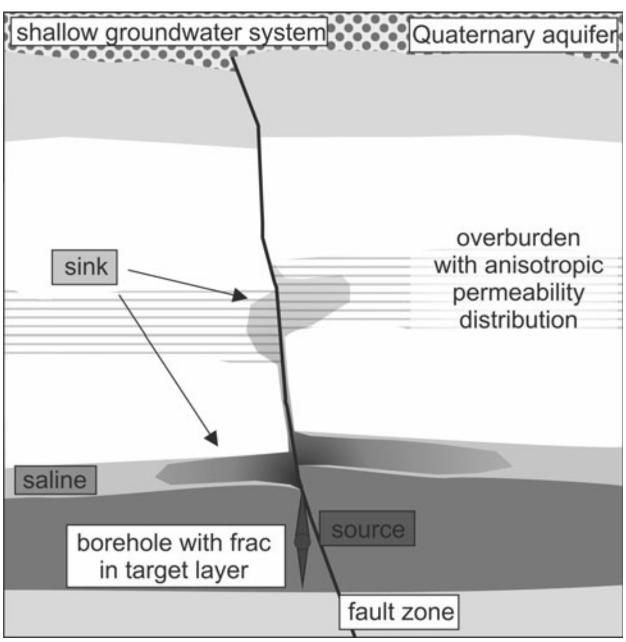

Fig. 3 Conceptual model of the system components for the risk assessment. The figure shows a vertical cross section perpendicular to a horizontal borehole

Definition of type settings at local scale

In order to account for the local variability of hydrogeological characteristics and still to be able to generalize the outcomes of the modelling procedure, the characterisation and modelling activities concentrate on different so-called hydrogeological settings that:

- Describe the spectrum of local geological and hydrogeological features, such as aquifer and barrier rock formations;
- Account for the local geological and hydrogeological variability;
- Reduce the flow system to those elements relevant for the migration process;
- Provide the basis for an efficient modelling process.

The variables for the definition of the settings considered include:

- Regional attribution;
- Thickness of overburden;
- Presence of sealing salt formations.

The respective settings also required detailed geological data, which is why the settings are generally associated with the presence of an existing borehole or geologic profiles in a high resolution. Tables 1 and 2 summarize the main characteristics of the hydrogeological settings that formed the basis for the modelling process.

Table 1 Characteristic type settings in the Münsterland Cretaceous Basin. In Fig. 1 the approximate position of the sites is indicated

	Faulted	Unfaulted
Low thickness of overburden	Bad Laer (≈500 m)	Borken (≈800 m)
Large thickness of overburden		Nordwalde (≈1,400 m)

Table 2 Characteristic type settings in the Lower Saxony Basin. In Fig. 1 the approximate position of the sites is indicated

	With evaporites	Without evaporates
Low thickness of overburden	Lünne (≈1,200 m)	Damme (≈1,300 m)
Large thickness of overburden	Quakenbrück-Ortland (≈2,400 m)	
Very large thickness of overburden	Vechta (≈3,700 m)	

Transport at regional scale

The two different regional areas are also distinct with respect to their geological architecture and in particular their hydrogeological flow system (cf. Paragraph Geological and hydrogeological characterization). While the MCB is characterized by a pronounced hydrogeological system in the Cretaceous Cenomanian–Turonian carbonate sequence, regional flow can be assumed to be negligible in the LSB because of its undifferentiated (flat) topography.

Definition of scenarios

It was already discussed, how the different model scenarios depend on the actual processes and conditions in the reservoir or the overall geological system, and the actual stage in the lifetime of a site. Three scenarios were selected for the illustration of the migration of the fracking fluids and methane.

Scenario 1 describes a short-term, local-scale upward flow phase of the fracking fluids due to the high-pressure gradient imposed during the fracking operation (2 h duration plus ca. 10 h of pressure relief and recovery phase). The fluids migrate into a geological overburden material, intersected by a permeable vertical fault zone. The overburden allows for anisotropy effects, i.e. fluid flow can occur preferentially horizontally parallel to the maximum permeability vector in the horizontal direction (differing from the vertical by several orders of magnitude).

Scenario 2 simulates the long-term, regional-scale transport within the deep carbonate system of the MCB, driven by the regional hydraulic gradient from the Teutoburger Wald southwards. Fracking fluids are assumed to enter directly into the groundwater system, i.e. no barrier formation is accounted for between the top of the frac and the deep groundwater system, following the general philosophy of assuming unlikely, highly unfavourable, but still physically feasible conditions. Furthermore, the regional carbonate flow system is intersected by a hydraulically highly conductive fault zone (conductivity corresponds to shallow conductivity of a permeable fault zone; at depth, the pathways tend to be closed, resulting from high lithostatic stresses).

In scenario 3 the long-term migration of methane into shallow geological layers driven by gravitational and capillary forces is simulated.

Monitoring concepts, base line definition

Federal as well as regulators of the German States defined standardized monitoring measures according to EU Water Framework Directive. Focus is the observance of environmental objectives and the detection of trends. Causes for adverse effects are to be determined as well as measures for rehabilitation and prevention. The foundation of a reasonable monitoring concept will be a statistically verified baseline documenting the pre-development conditions (geogenic and anthropogenic background concentrations) in the vicinity of a planned site. Osborn et al. (2011) showed the importance of this step for the Marcellus and Utica shales (Pennsylvania), where elevated methane concentrations together with thermogenic signatures correlate with the distance to production wells and are probably related to leakage problems in the tubing system. However, no survey has been conducted to collect the necessary pre-development baseline information.

Geological and hydrogeological characterization

Regional hydrogeology of the study areas

Geology and hydrogeology of the Münsterland Cretaceous Basin (MCB)

The MCB is bounded by the Osning (Teutoburger Wald) in the north, the Eggegebirge Mountains in the east and in the south by the Haarstrang ridge north of the Sauerland area. In the west the basin opens to the Lower Rhine Bay as well as to the Central Netherlands Basin. In the central and eastern part of the MCB three main hydrogeological units comprise the section of the overburden: the Cretaceous Cenomanian–Turonian Aquifer (CTA) that overlays the Carboniferous, the thick hydraulic barrier sequence of Cretaceous Coniacian to Senonian marlstones ("Emscher Mergel" facies), and the Quaternary unconsolidated sediments including the stress relieved, fractured, near-surface weathering zone of the Emscher Mergel. Only in the western parts of the MCB a mixed succession of Triassic sediments of the Bunter Sandstone contribute to the barrier function of the overburden. Along the basin, circular strip of the outcropping CTA karstification is widespread, which—based on increasing salinities—decreases towards the centre of the basin. Except for the Quaternary cover sediments the overall structure corresponds to a closed syncline with a low-angle inclination in the south and steep inclinations or overtilting in the north (Osning fault system). While the near-surface groundwater is drained to the west (Lippe catchment) and to the northwest (Ems catchment), there is virtually no information available based on in situ observations about the deep groundwater system, especially in the CTA. One assumption, however, is that due to the higher groundwater potentials at the northern basin boundary the deep regional groundwater flow is directed south to southwestward. Hence, the occurrences of springs with elevated salinities below the outcropping interface of the CTA and the "Emscher Mergel" could be at least partially a result of the assumed deep flow system. The sources of salinity in groundwaters of the MCB are still not well understood (cf. e.g. Grobe et al. 2000; Grobe and Machel 2002). In general, the salinity in the MCB continuously increases with depth.

Because a regional, lateral transport of groundwater contaminants to the south would impose an additional risk for example for therapeutic spas that have a long tradition especially in the south of the MCB, the described scenario was considered in this study according to its conservative approach. While a regional hydraulic gradient between the northern and southern boundaries can be approximated to 4.4×10^{-6} based on spring locations and elevations along the basin boundary the estimation of the effective hydraulic conductivity remains a difficult task because neither the primary salinity of the source nor the discharge can be determined with sufficient accuracy. Applying rough estimates of discharge volumes of saline groundwater from Michel and Struckmeier (1985) and Struckmeier (1990), a hydraulic conductivity of 2.8×10^{-6} m/s was calculated (Sauter et al. 2012) and eventually applied in the transport simulations. However, this value is believed to range much above those of the actual field conditions in the central deep section of the MCB for several reasons.

On the one hand, the CTA in the central section would feature a considerable degree of karstification. On the other hand, salinities are high and mixing with fresh water carrying relevant amounts of dissolved CO_2 is not to be expected. The same applies to other sources of CO_2. The saline springs and groundwater of Bad Westernkotten south of Lippstadt, where significant concentrations of CO_2 are detected are related to the basement arch structure of Lippstadt. Here, the geological situation is different compared to the locations investigated in the central parts of the basin, where the thickness of the coal-bearing Upper Carboniferous reaches up to 3,000 m, while it is absent in the Bad Westernkotten area.

Due to the regional distribution of the Cretaceous Emscher Mergel facies, which is only locally and in its weathered, upper part a minor source for groundwater, the available high-yield groundwater aquifers are strongly protected, such as the deeply incised Pleistocene Münsterland channel or the limited distribution area of the Upper Santonian to Lower Campanian Halterner Sandstone facies, which in the western parts of the MCB partially replaces the Emscher Mergel facies. Other partially productive aquifers are located in Pleistocene sands and gravels of the Sandmünsterland in the north and north east of the MCB.

Indicators for upflow of deep groundwaters in the Münsterland Cretaceous Basin

A main feature of the hydrogeological system of the MCB is the existence of saline to highly saline groundwaters in the deeper sections of the basin. Despite a minor number at the northern basin boundary, most of the historical saline springs of the MCB discharged along a southern spring line, where the outcropping CTA submerges below the "Emscher Mergel" and confined conditions prevail. However, several of the formerly known springs of varying salt concentrations of generally less than 90 g TDS/L have become less saline due to the production of saline water for thermo-saline spas during the last 200 years (Struckmeier 1990). Due to groundwater drawdown in the coal mining area in the southwestern part of the MCB, the previously existing saline springs west of Unna dried up. Fluctuating discharge rates and salinities in the course of stronger precipitation events or periods were observed early on [Huyssen 1855; Michel 1983 (quotes Keferstein 1823); Struckmeier 1990]. Although of major importance for the applied balance calculations within this study, there still is high uncertainty in the scientific community about the salinity levels in the deep sections of the CTA, because no depth-level-oriented sampling was performed in the few deep boreholes that were drilled in the past (Michel 1983). No such data are available even since 1983. In order to account for this deficit, model-salinities have to be defined. In accordance with the overall conservative approach of this study a model-salinity of NaCl = 100 g/L for the deep saline CTA was assumed in the numerical models, which is close to the maximum known values in the concentration records of historical and actual spring discharge. Much higher salinities of up to 210 g/L were observed during water influx into active coal mines (Wedewardt 1995).

Methane is a well-known component in groundwaters of the MCB (e.g. Melchers 2008; Strobel and Wisotzky 2009). While in the past the origin of the methane was highly speculative, Melchers (2008) first thoroughly investigated the formation, migration, and risk potential of the observed methane in the MCB. He found no clear evidence for distinct isotopic signatures that would clearly indicate a thermogenic origin of the methane. The majority of methane concentration values are below solubility limits. Instead, except for very few cases, the methane and other indicators involved in the formation process have a distinct biogenic fingerprint. Possible methanogenic pathways that are likely to prevail in the investigated hydrochemical environments are acetic fermentation but also reduction of CO_2 and are assumed to originate from hydrogeochemical processes within the Emscher Mergel (marlstone) sequence itself. Usually higher methane concentrations in the saturated Quaternary layers immediately above the Emscher Mergel and reduced sulphate contents probably due to methane oxidation support the above assumptions (Strobel and Wisotzky 2009). However, the chemical and isotopic signature represent important indicators to identify additional thermogenic methane fluxes related to gas production from unconventional CBM reservoirs. Osborn et al.

(2011) have successfully shown that the approach of hydrochemical and isotopic fingerprinting can be applied as an essential part of a monitoring concept. However, more recent systematic investigations (e.g. Grobe et al. 2000; Grobe and Machel 2002, or Voigt et al. 2007) indicate that although the main hydrochemical characteristics and components of the MCB can be traced, the specific kind and distribution of the sources of salinity, pathways for migration, and water–rock processes are still highly variable and uncertain.

Geology and hydrogeology of the Lower Saxony Basin (LSB)

The LSB represents the southwestern (Lower Saxony) subbasin of the NGB. The investigated exploration areas are distributed from west to east approximately from Lünne to Wunstorf and in north–south direction approximately from Vechta to the same latitude as Osnabrück. On its south side the Niedersachsen Tectogene (Osning/Teutoburg Forest—Wiehengebirge Mountains) separates the LSB from the MCB. North of the Pyrmont–Piesberg axis the Variscan basement rapidly dips below a thick sequence of Upper Permian to Quaternary. The post-Variscan sedimentary sequence reflects differential subsidence rates, spatially varying halo-tectonic stresses, as well as the Late Cretaceous to Early Paleogene inversion tectonics especially at the southern basin boundary (Drozdzewski 1988). The latter process resulted in relative block movements during which the Lower Saxony Tectogene was uplifted.

The rapidly increasing thickness of the unconsolidated Cenozoic sediments accompanied by a rather undifferentiated topography suggests regional small hydraulic gradients (Lbeg 1991), which are irrelevant with respect to the reasonable time scales considered in the risk assessment process. Usually freshwater resources are abstracted from depths of less that 100 m bgl. However, local resources reach down to depths of 300 m. This already represents a zone of limited exchange with surface-near groundwater, where the transition to stagnant conditions and increased salinities is continuous (Hahn 1991). Because of the complex genesis and distribution of the Cenozoic sediments and the in general relative small overall thickness compared to the complete geological profile integral values were assumed for the model parameters of the numerical simulations. Similarly to the MCB, Pleistocene deeply incised channels represent important groundwater aquifers of high-yield.

Indicators for upflow of deep groundwaters in the Niedersächisches Becken

In general, groundwater salinisation phenomena in the LSB and the NGB are observed in zones of pressure release, i.e. in the close vicinity of larger streams; and no fresh groundwater resources are to be found at depths below 300 m (Lbeg 2012). Detailed studies about possible salinisation mechanism in the LSB and NGB are provided by Huenges et al. (1997) and Klinge (1991). In comparison to the northern parts of the NGB the area affected by salinisation is rather small in the investigated parts of the LSB and primarily limited to the Quakenbrück basin (Lbeg 2012). The known chloride concentrations in groundwater from the database of the NIBIS map service provide a unique, spatially undifferentiated value of more than 250 mg/L. The Quakenbrück basin is a typical Pleistocene erosive structure of a glacial tongue of the Saale complex (Streif et al. 2007). Older deeply incised channels of the Elster glacial period are preserved as well. However, if salinisation occurs generally only the deeper parts of the Pleistocene channels in the LSB or NGB are affected. According to Lbeg (2012) two salt pillow structures exist in the Quakenbrück area. But it is unknown, whether they are the direct cause for increased salt concentrations or if permeable faults are involved. However, as long as the integrity of the deep salt formations is not substantially disturbed, the effectiveness of this important barrier rock will be preserved.

Regional conceptual model and geometries

The available geological information from published borehole logs and geological maps was conceptualized by defining the main geological units and constructing cross sections as a prerequisite for modelling. For the western and central part of the MCB two NW–SE directed geological and hydrogeological cross sections were constructed. Figure 4 shows the example of the hydrogeological cross section for the central part of the MCB. As no regional hydrogeological modelling was conducted in the LSB, only two NE–SW directed geological cross sections were created (cf. Fig. 1; Sauter et al. 2012).

Hydrogeological settings: local-scale geology and hydrogeology

As representative for various geological type locations in both, the MCB and LSB characteristic settings were defined associated with existing boreholes or based on geological data of the state geological surveys (Tables 1, 2). This approach not only considers the geological and hydrogeological specifics in the vicinity of a type location. It also ensures the coverage of a broader range of situations and in turn enables to generalize results and to detect investigation demands for other types of settings that were not covered in this study.

In the following, the lithologies of the penetrated units in the investigated regions are described in general without

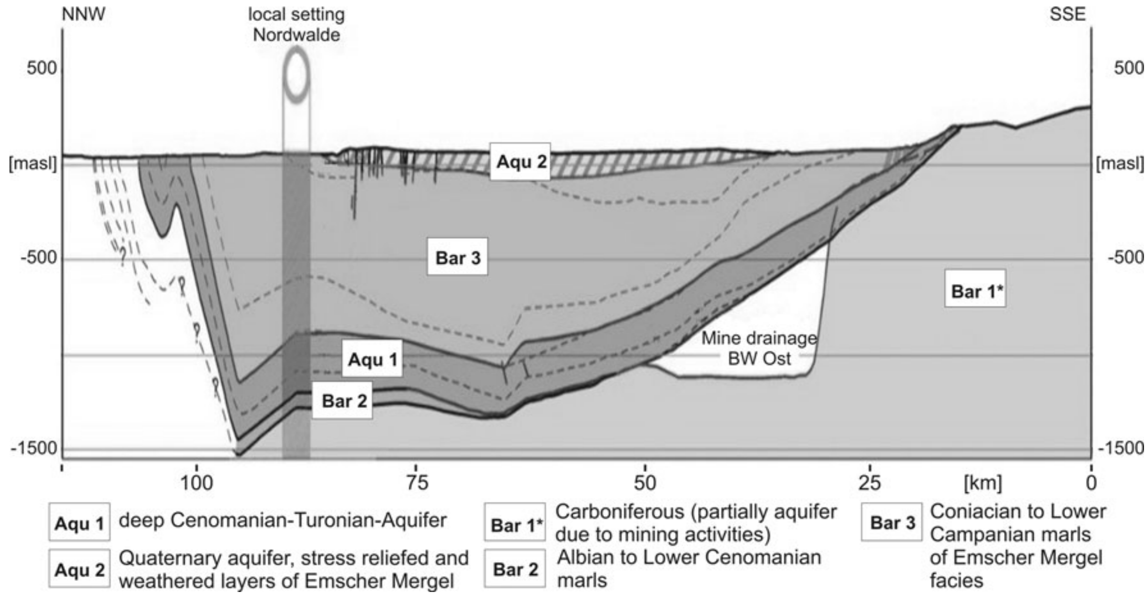

Fig. 4 Hydrogeological cross section *A–B* for the central part of the MCB

going into the local details. To respect proprietary rights all values given for thickness or depth are rounded.

Münsterland Cretaceous Basin

The coal beds of the Upper Carboniferous represent the target horizon in the MCB. In general, Permian to Triassic sediments are absent in the MCB. Only at the setting Borken in the western part of the basin Bunter Sandstone layers of primarily sandstone to shale and secondarily evaporates (anhydrite in the Röt formation Upper Bunter Sandstone formation) were deposited. Thin sections of Zechstein dolomite prevailed in both, setting Borken and Bad Laer. But all three settings comprise the same Cretaceous sedimentary succession that is overlain by unconsolidated Quaternary deposits of different thickness. While the Albian is characterized by shales and marlstones, the Cenomanian–Turonian sequence predominantly comprises limestones and limestone–marlstone alternations. The thick succession of Coniacian to Santonian predominantly marlstones, with secondarily limestone intercalations represent the Emscher Mergel facies. Thus, the main barrier rocks in the MCB are provided by the units of the Zechstein, Bunter Sandstone, Albian and Emscher Mergel. The Cenomanian–Turonian limestones represent the deep saline groundwater aquifer (CTA). Table 3 lists the thickness distribution at the individual settings.

Lower Saxony Basin

Due to the more complex geological history of deposition as well as differential movements or subsidence rates, respectively, the variation in distribution and thickness of the documented stratigraphic units in the investigated region is much larger that in the MCB. Thus, the individual profiles of the settings cannot be simplified in the same way as for the locations in the MCB. However, target horizons are the Lower Jurassic Posidonia shale (Lünne, Quakenbrück-Ortland), the Lower Cretaceous Wealden (Damme), and the Upper Carboniferous (Vechta, tight-gas). The thickness of the unconsolidated Quaternary sediments is ≥50 m. In turn, except for the setting Vechta were in addition thick Permian and Triassic layers including evaporite sequences were penetrated, the consolidated overburden comprises all kinds of Jurassic to Tertiary sediments. The majority of these are assigned to as barrier

Table 3 Penetrated thickness of the Upper Carboniferous and the overburden in boreholes in the setting areas of the MCB

Stratigraphic unit	Borken Thickness in [m]	Nordwalde Thickness in [m]	Bad Laer Thickness in [m]
Quaternary	25	10	<10
Coniacian to Santonian	175	940	Not existent
Cenomanion/ Turonian	200	350	300
Albian	50	100	150
Bunter Sandstone	350	Not existent	Not existent
Zechstein	10	Not existent	10
Upper carboniferous (not fully penetrated)	150	700	1,400
Total	960	2,100	1,900

rocks, such as shales, marlstones, and especially Upper Jurassic evaporite sequences.

The individual geological profiles may be taken from the final report of the workgroup (Sauter et al. 2012).

Hydrogeology of barrier and aquifer rocks

Based on a comprehensive literature research about effective hydraulic parameters of rock types existing at the investigated local settings, model parameters were derived. If applicable, particular attention was paid to the selection of data from literature sources dealing with safety aspects and with lithological units in the study area itself. For example, intensive research is conducted to evaluate the effectiveness of shales, mudstones, and salt formations as barrier rocks for deep repositories for hazardous waste or for injection horizons for supercritical CO_2. Especially barrier rocks such as the thick sequence of Coniacian to Lower Campanian marlstones in the MCB (local name: Emscher Mergel) and mudstone and rock salt in the LSB were given particular attention with regard to its characterisation since they represent the main barrier for fluids migrating from the target zone to the shallow groundwater system. A prevailing problem is that only few surveys focus on larger depths and bulk properties resulting from large-scale experiments. However, the considered literature data were evaluated based on the documented depth, i.e. less or more than 300 m bgl. Additional weighting was given based on the applied techniques that determine the representativeness of the measurements (e.g. pumping tests, core tests in triaxial cells, etc.). Honouring the conservative approach of this study, the unfavourable margins of the ranges of permeability and porosity were selected. In Table 4, the final compilation of generic effective hydraulic parameters for the distinguished lithological rock types is presented. The main groups distinguished are aquifer and barrier.

Table 4 Compilation of default hydraulic parameters for aquifer and barrier rock types present in the MCB and the LSB based on literature sources (cf. Paragraphs Aquifer rocks and Barrier rocks)

Rock types	K_f		N_e
	<300 m bgl [m/s]	>300 m bgl [m/s]	[−]
Quaternary	1×10^{-4}		0.2
Sandstone	1×10^{-6}	1×10^{-8}	0.05
Limestone	1×10^{-5}	1×10^{-7}–1×10^{-6}	0.01
Shale/mudstone	1×10^{-7}	1×10^{-9}	0.001
Marlestone	1×10^{-6}	1×10^{-9}	0.001
Evaporites		1×10^{-11}	0.001

K_f and n_e represent hydraulic conductivity and effective porosity, respectively

Aquifer rocks

Strongly depending, for example, on depth, genesis and facies, karstification, or fracture density limestones, dolomites, and sandstones can build up important aquifers.

A prominent example for a limestone aquifer in the investigation areas of the MCB is the fractured CTA. While highly conductive due to karstification in the outcropping areas, the permeability and degree of karstification decrease towards the basin centre. The spectrum of effective hydraulic conductivities and effective porosities of *limestones* derived from various literature sources ranges from 10^{-8} to 10^{-4} m/s and 0.005 to 0.015, respectively (Baltes 1998; Bundesamt für Strahlenschutz 2009; Reutter 2011; Rudolph et al. 2008). However, the Zechstein dolomite is rather a barrier rock of low conductivity and effective porosity. The high permeabilities and high porosities provided by Reutter (2011) and Baltes (1998) represent limestones at shallow depths in Lower Saxony and in the reach of mining activities, respectively.

Sandstones are much more widely spread in the LSB than in the MCB. The spectrum of effective hydraulic conductivities and effective porosities of sandstones derived from the considered literature sources range from 3×10^{-11} to 1×10^{-4} m/s and 0.01 to 0.05, respectively (Delakowitz 1996; Baltes 1998; Bundesamt für Strahlenschutz 2009; Reutter 2011; Langkutsch et al. 1998; NAGRA 2008). The hydraulic parameters naturally depend on grain size distribution, fracture density, diagenetic and compaction processes. While higher permeabilities and higher porosities are expected at shallow depths, or in the reach of mining activities that loosen the overburden, increasing depths are accompanied by decreasing parameter values.

Barrier rocks

The main barrier rock types in the MCB are marlstones, while shales, mudstones, and evaporates are dominating in the LSB

Mudstone and shale The evaluated literature sources focussing on mudstone and shale give parameter ranges for hydraulic conductivities and effective porosities at different depths of 1×10^{-16} to 1×10^{-7} m/s and 0.001 to 0.072, respectively, for various lithostratigraphic units at different locations worldwide (Gautschi 2001; Neuzil 1994; Croisé et al. 2003; Hekel 1994; Röttgen 2004; Appel and Habler 2002; Bundesamt für Strahlenschutz 2009; Langkutsch et al. 1998; Goens 2011; Reutter 2011). For shallow depths Appel and Habler (2002) even report comparably very high hydraulic conductivities of up to 1×10^{-6} m/s (<200 m bgl). However, at depths below 300 m bgl conductivities are generally lower than 10^{-9} m/s.

Marlstone Similar hydraulic properties, such as mudstones and shales are characteristic for marlstones, which, compared to the other ones, have varying contents of carbonate and potentially higher proportions of non-clay-size components. According to the evaluated literature sources the range of hydraulic conductivities and effective porosities is 1×10^{-11} to 5×10^{-6} m/s and <0.001 to 0.03, respectively (Baltes 1998; Thielemann 2000; Rudolph et al. 2008; Appel and Habler 2002; Delakowitz 1996; Langkutsch et al. 1998; Reutter 2011). While in shallow levels hydraulic conductivities may reach 5×10^{-6} m/s, values decrease to equal and less than 1×10^{-9} m/s at depths below 300 m bgl. Based on large-scale water balance calculations for the MCB Struckmeier (1990) estimated a reasonable range for the marlstones of the Emscher Mergel between 1×10^{-11} and 1×10^{-9} m/s.

Evaporites Evaporite sequences are considered as barriers of high effectiveness, which is one reason why they are investigated as potential host rocks for nuclear waste repositories in Germany (e.g. Gorleben, Morsleben). As the evaluated literature sources all confirm an upper limit for hydraulic conductivities of 1×10^{-11} m/s (Bundesamt für Strahlenschutz 2009; Bornemann et al. 2008; Langkutsch et al. 1998), this upper limit was selected as default value together with a default effective porosity of 0.001.

Parameterization of the lithological model units

To reduce complexity and discretisation demand in the numerical models to an appropriate level zones of similar hydraulic properties or typical high frequent rock type alternations were aggregated to packages or model material units. While intrinsic hydraulic anisotropies cannot be assigned to those, macroscopic anisotropies were preserved by thickness-weighted harmonic and arithmetic means for vertical and horizontal conductivities, respectively (e.g. Jang et al. 2011). If not applicable in detail, the highest and the lowest hydraulic conductivities of the lithological succession were assigned to the horizontal and the vertical hydraulic conductivities of the aggregated model units, respectively. Whenever possible, weighted arithmetic averages for porosity have been calculated as well according to Satter et al. (2008).

Fault zone effects on fluid flow

Fault zone characterization in the Münsterland Cretaceous Basin

A chloride-mass-balance approach was developed to estimate the hydraulic properties of potential fault zones in the MCB. It is based on the conservative assumption that all salinity is caused by upflow of highly saline water from the deep confined CTA through fault zones that mixes with unaffected shallow groundwater ($Cl^- = 12.5$ mg/L). As discussed above, the exact value of the salinity of the saline end member is unknown, and part of the observed elevated surface-near groundwater salinity may be related to connate fluids in the Emscher Mergel. But because the contribution of the latter can hardly be estimated, the applied model concentration of $Cl^- = 50$ g/L was entirely assigned to the CTA and is based on historical records of spring salinities, borehole observations, and groundwater leaking from the overburden into the coal mines (cf. discussion about indicators of deep groundwater upflow (this issue), or in Sauter et al. 2012). The regional hydraulic gradient for the CTA was estimated to 4.4×10^{-4}. Using official hydrogeological maps and commentaries (Geologischer Dienst Nordrhein-Westfalen 1997, 1981, 2006) and a regional shallow groundwater contour map (provided by Agency for Nature, Environment, and Consumers of North Rhine-Westphalia) necessary information about salinities in and the local effective saturated thickness of the permeable portions of the shallow groundwater system, as well as local hydraulic gradients at the investigated local settings could be collected. After determining the shallow groundwater fluxes at the local settings, the equivalent fault zone transmissivities can be derived by Eqs. 1 and 2:

$$\left(T_{\text{fault}} = \frac{Q_{\text{fault}}}{\text{gradh}_{\text{fault}}}\right) \tag{1}$$

$$\left(Q_{\text{Quaternary}} + Q_{\text{fault}}\right) \cdot C_{\text{mix}} = Q_{\text{Quaternary}} \cdot C_{\text{Quaternary}} + Q_{\text{fault}} + C_{\text{fault}} \tag{2}$$

with Q the discharge rate, C the Cl^- concentration, gradh the local gradient, and T the fault zone transmissivity. Equation 2 simplifies as we can replace the unknown discharge rate in the fault zone (Q_{fault}) by the product of the remaining unknown of the fault transmissivity (T_{fault}) and the local head gradient ($\text{gradh}_{\text{fault}}$).

Fault zone characterization in the Niedersächsisches Becken

Brace (1980) compared permeabilities of fractures, fractured bulk rock, and large-scale phenomena of crystalline and argillaceous rocks at different scales and depths. The results showed that for the investigated argillaceous barrier rocks, such as shales or clay-rich sediments faults permeabilities do not exceed 10^{-16} m². Another comprehensive study of Jolley et al. (2007) that also considers other studies clearly indicate that with increasing depths and relevant clay contents (>20 %) effective fault zone permeabilities will not be larger than 10^{-16} m². With 50 % clay content the permeability reduction is 2 orders of magnitude. Thus, the default permeabilities of potential fault zones were assumed to be 10^{-16} m^2. In places of thick salt formations the default permeability was set to 5×10^{-18} m^2, i.e. five times the assumed permeability of salt rock based on the conservative approach (c.f. Table 4).

Results and discussion

Evaluation of the generalized approach

A conservative, physics-based approach to assess the risks in the geological system in the context of hydraulic fracturing operations was chosen to describe and simulate the main system components, migration pathways of fracking fluids and methane, and relevant time and spatial scales in different phases of the lifetime of an unconventional gas reservoir. The pronounced conservative strategy aimed to define the conditions at potential production sites, which would determine the limits of the geological and hydraulic plausibility for the investigated system. The strategy that was followed was the superimposition of very unfavourable assumptions in the conceptual model of the hydrogeological system. Beside the implementation of unfavourable geometries (like permeable faults that connect the source (frac) of the fluids and the hydraulically conductive horizons above) or highest, but still plausible permeabilities, the conservative approach was amplified by simulating the migration processes additionally using unfavourable boundary conditions (e.g. upkeep of maximum injection pressure despite significant loss of fracking fluid) and not considering "retarding" processes such as matrix diffusion, sorption, and biodegradation that naturally exists.

Although the simulation results are expected to vastly overestimate transport distances likely to be observed in nature, they provide safe measures to define minimal distances between the tubing used for the hydraulic fracturing operation on the one hand and the surface or a protected deep groundwater aquifer on the other hand. The definition or selection, respectively, of local type settings turned out to be a valuable approach on the one hand to consider the specifics of an investigated location, and in addition by studying a broader spectrum of geometries and hydraulic parameters to cover a range of constellations in the investigated region. It provides a method of risk assessment applicable for comparable settings with similar characteristics and to generalize results.

Specific results for the MCB and the LSB

The geology and hydrogeology of the exploration areas in the MCB and the LSB were described and characterized to reproducibly define the required main system components, pathways, and relevant scales for the risk assessment. Based on a systematic approach, the system geometries and components were parameterized on local and regional scale. The high-resolution lithological logs were aggregated to appropriate model units, while the macroscopic hydraulic anisotropy was preserved. Although available information about the hydraulic effectiveness of faults in the MCB and LSB is rare, the two specific approaches for the MCB (chloride mass balance) and the LSB (analogue studies) to parameterize potentially existing faults are comprehensible and respect available site-specific data. The main findings of the conducted simulations for the studied local and regional settings are presented in short according to the scenarios that were set up. A detailed discussion, however, is provided in Kissinger et al. (2013, this issue).

Scenario 1 (local-scale vertical migration of fracking fluids)

The simulations show rather limited vertical migration distances at the local settings. In case of the setting Bad Laer, where high fault zone permeabilities were assumed, values of up to 50 m are reached. Due to the pronounced conservative approach and as opposed to fracking operation conditions, where in case of significant fluid loss into a high permeable fault zone the shut off of pumps would be triggered, results are expected to be overestimates. In turn they provide recommendable safe minimum distances.

Scenario 2 (regional-scale migration of fracking fluid in the MCB)

In addition to a small regional hydraulic gradient, a vertical gradient from the CTA to the surface-near groundwater system exists. Depending on the strength of the latter and the applied permeability of the assumed fault zone, which was implemented in the model very close to the position upstream of the plume of fracking fluid in the CTA, the contaminants migrate vertically. Only in the case of the highest assumed fault permeability and vertical hydraulic gradients the contaminants may reach the surface-near groundwater system. The lateral migration amounts to values of several metres to 25 m per year, depending on the selected conditions.

However, the lateral contaminant migration will be certainly overestimated due to the unconsidered processes of matrix diffusion, sorption, and biodegradation of the organic compounds of the fracking fluids. Although the overall risks can be classified as small a priority list for further necessary investigation is provided with the recommendations.

Scenario 3 (local-scale migration of methane)

The simulation results, discussed in detail in Kissinger et al. (2013, this issue) indicate that only under specific model conditions following the pronounced conservative approach relevant volumes of methane would escape to the atmosphere as in the case of the setting Lünne. The essential controlling factors are the existence of salt formations, permeable faults, low residual gas saturations together with small effective porosities, the remaining mobilizable volume of methane, the chosen boundary conditions at the base of the model, and the thickness of the overburden. When the assumed fault permeability in the domain of the salt formation at the setting Lünne was set to an appropriate value taking into account the self-healing effects caused by the rheology of pressurized salt, the exhalation of methane becomes insignificant. Also the constant rate of methane migration into the overburden at the lower boundary is unlikely to be observed in nature.

Summary and recommendations

To assess the risks for the geological system and the surface-near groundwater system in particular in the context of hydraulic fracturing operations a pronounced conservative, physics-based approach was chosen. The conservative character is defined by determining the limits of the geological and hydrogeological plausibility for the investigated system by superimposing unfavourable assumptions in the conceptual and numerical model. The methods to define the model geometries and the spatial distribution of the model parameters were designed to be comprehensible and reproducible. On the one hand, the developed strategy to describe and characterize the main system components, migration pathways of fracking fluids and methane, and relevant scales during different phases of the reservoir lifetime is specific (local type settings) with respect to the investigated exploration areas and local sites. On the other hand, it provides a reasonable concept to analyse a broader spectrum of geometries and parameters that covers similar geological settings and allows to generalize results in a specific region but also between different regions.

Recommendations

Minimum distances

Figure 5 generalizes the simulation results for the MCB and the LSB in terms of a minimum distance of ca. 1,000 m between the casing perforation location and the surface. It is based on the results of (a) the field study of Fisher and Warpinsky (2011) that determined maximum fracture heights of 500 m; (b) the study presented here together with Kissinger et al. (2013, this issue) that found maximum vertical migration distances of 50 m, which if the frac was pressurized a second time from a neighbouring borehole increase to 100 m, and finally sum up to 200 m applying the rule of double safety. As defined in the concept of the presented study (c) the top 300 m are assumed to be increasingly permeable due to stress relief at shallow horizons and are therefore not considered as a barrier.

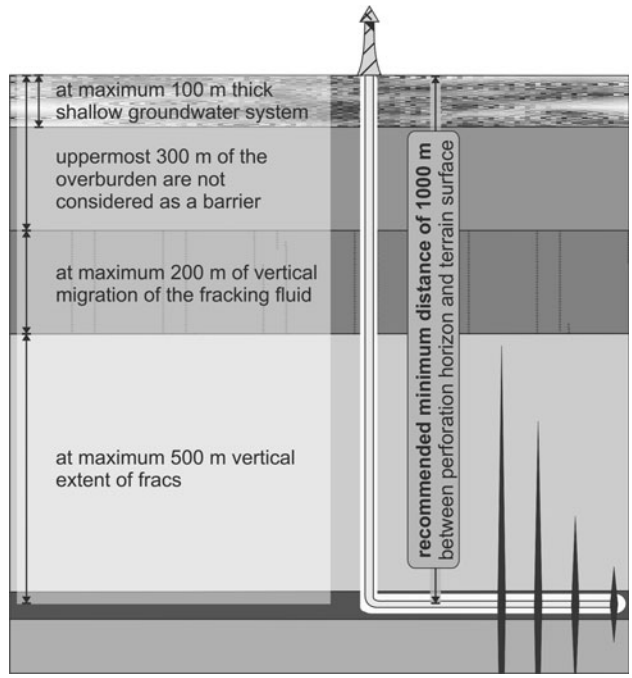

Fig. 5 The figure illustrates the recommendation for minimum distances between the surface and the location of the casing perforation

Between the perforation in the casing and the base of a protected deep aquifer a distance of 600 m is suggested, which, in addition to 500 m of maximum frac height, assumes a single maximum migration distance of 25 m that in analogy to the definition of the overall migration component above sums up to 100 m. The lower maximum migration distance of 25 m, compared to 50 m is based as well on the study presented here together with Kissinger et al. (2013, this issue). It is a reasonable but still conservative assumption, since faults of high and constant permeability of 9.1×10^{-14} m^2 are not likely to exist at depths considered here.

Should knowledge about a specific region be available at sufficient quality and detail to limit the range of possible geometries, parameters, or operational conditions, minimum distances have to be determined with respect to the actual investigated geological system.

Monitoring

Any realization of sites for unconventional gas production must be in accordance to the EU Water Framework Directive (EU-WFD) implemented by the German regulators. This also implies the set up of a comprehensive database in places, such as the MCB, where coal mining and exploration activities already caused complex effects in the geological system. To achieve the environmental objectives defined by the EU-WFD, a statistically verified baseline documenting the environmental pre-development conditions and an appropriate monitoring concept, including preventive and measures for rehabilitation is required. With respect to the baseline it is recommended to assess the geological as well as anthropogenic background concentrations of substances that potentially could harm humans and the environment or that can serve as indicators for migration processes in the vicinity of the production site. To clearly differentiate between pathways during the monitoring ideally sets of indicator substances should be defined that are exclusive components of (a) fracking fluids and derived metabolites and (b) mobilized brines and methane (chemical and isotope signatures). In addition to a set of groundwater monitoring wells in the vicinity of a drill site it is suggested to instal a well as close to the gas production well as technically possible. Its filter should be positioned in the lower (if exists) exploitable groundwater horizon. On the one hand, the sampled groundwater there can provide a site-specific baseline for all relevant parameters. On the other hand, the well would be used to create a depression cone around the gas production well allowing early detection of changes in the water quality and at the same time providing a representative sample of an integrated volume. In case of any disturbances at the drill site the suggested well could function as a protection well. The overall monitoring plan may be subdivided in phases according the to the main stages of the lifetime of the reservoir.

Research

The conducted study showed that further research is required to fully understand the relevant processes to improve the assessment of risks. Among others, the highest demand is related to the estimation of residual gas saturation and the release mechanisms of methane in the post-production phase, and the characterization of barrier rocks and faults especially between 1,000 and 100 m as this domain was only of small scientific interest in the past. If hydraulic fracturing would be applied on a larger scale in Germany the technical and economical optimization of hydraulic fracturing in shale or coal beds surely would be of interest as well.

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