SPECIAL ISSUE

Hydraulic fracturing in unconventional gas reservoirs: risks in the geological system, part 2

Modelling the transport of fracturing fluids, brine and methane

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Abstract Hydraulic fracturing is a method used for the production of unconventional gas resources. Huge amounts of so-called fracturing fluid ($10,000$–$20,000$ m^3) are injected into a gas reservoir to create fractures in solid rock formations, upon which mobilised methane fills the pore space and the fracturing fluid is withdrawn. Hydraulic fracturing may pose a threat to groundwater resources if fracturing fluid or brine can migrate through fault zones into shallow aquifers. Diffuse methane emissions from the gas reservoir may not only contaminate shallow groundwater aquifers, but also escape into the atmosphere where methane acts as a greenhouse gas. The working group "Risks in the Geological System" as part of ExxonMobil's hydrofracking dialogue and information dissemination processes was tasked with the assessment of possible hazards posed by migrating fluids as a result of hydraulic fracturing activities. In this work, several flow paths for fracturing fluid, brine and methane are identified and scenarios are set up to qualitatively estimate under what circumstances these fluids would leak into shallower layers. The parametrisation for potential hydraulic fracturing sites in North Rhine-Westphalia and Lower Saxony (both in Germany) is derived from literature using upper and lower bounds of hydraulic parameters. The results show that a significant fluid migration is only possible if a combination of several conservative assumptions is met by a scenario.

Keywords Fracturing fluids · Methane · Modelling

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Introduction

The production of unconventional gas resources which require a hydraulic fracturing process to be released, such as shale gas, has become an economically attractive technology for a continued supply of fossil-fuel energy sources in many countries. Recently, a major focus of interest has been directed to hydraulic fracturing in Germany. The technology is controversial since it involves severe risks. The main difference in risk with respect to other technologies in the subsurface such as carbon sequestration is that hydraulic fracturing is remunerative, and it is important to distinguish between economical and environmental issues. Within the framework of ExxonMobil's hydrofracking dialogue and information dissemination process (Ewen et al. 2012), the working group Risks in Geological Systems (Sauter et al. 2012) was tasked with the investigation of potentially hazardous events resulting from the

propagation of fracturing fluids and methane into shallow groundwater aquifers due to hydraulic fracturing activities.

This framework does not include a full-scale risk analysis at the current stage of work. Instead, it defines certain conservative scenarios which provide a broad range of expected damages due to different potential hazards.

Quantitative risk evaluation is beyond the scope of this work, since the probability of a given scenario and the variability of important model input parameters are not investigated. To determine potential hazards, it is necessary to first identify potential flow paths as well as the mechanisms which may lead to fluid migration. Based on these findings, scenarios are derived which can capture the relevant mechanisms while including system parameters from potential unconventional gas production sites.

The article by Lange et al. (2013) analyses the geological and hydro-geological conditions in the Münsterland Basin situated in the state of North-Rhein Westphalia and the Lower-Saxony Basin. Seven settings are set up with characteristic parameters for the areas which are in the focus of the study. The hydro-geological parameters of the seven settings are given in Online Resource 1. The simulations presented in this article are based on these settings and their parametrisation. The simulations are intended to show qualitatively the possible effects of hydraulic fracturing, for example, to identify critical combinations of parameters which may lead to a contamination of groundwater resources or, in the case of methane migration to, an increase in greenhouse-gas emissions. Hence, similar to a back-of-the-envelope calculation, the scenarios are kept as simple as possible. Nonetheless, due to the complex nature of the processes and/or geometries involved, a numerical model is extremely handy.

In light of an intended continuation of this work towards a thorough risk assessment, numerical simulation capabilities are indispensable. A further aim of this study is offering the opportunity to recognise gaps in knowledge and to point out a concise demand for further-more focused-research.

This paper comprises the following sections: "Identification of flow paths" gives a brief summary of possible flow paths; "Limitations, general aims and approach of the modelling activities" deals with the scope and aims of this work; in "Assumptions, scenario setup and results" the scenarios and the simulation result are discussed and in "Summary and conclusion" a brief summary as well as concluding remarks and the demand for further research are presented.

Identification of flow paths

In the following, possible flow paths of fracturing fluid and of methane will be discussed. These flow paths are shown in Fig. 1.

Flow paths of fracturing fluid and/or brine

F1 Flow through natural fault zones: The fractures created during the stimulation period could connect with a natural fault zone and the fracturing fluid could be forced through this fault zone as a result of the strong pressure buildup in the system (see Fig. 1). This pressure buildup diminishes as soon as the hydraulic fracturing operations (which may last for about 2 h) are stopped, and the flow ceases.

F2 Flow through leaky boreholes (well integrity problem): Fluids may leak into the freshwater aquifer through the borehole (e.g. due to a faulty installation). However, this would imply an incomplete sealing of the borehole annulus or the use of leaky cement.

F3 Spill at the ground surface: In the case of an accident, large amounts of contaminants may infiltrate into the aquifer. A continuous contamination of the aquifer is also possible if a leak occurs undetected.

Flow paths of methane

M1 Flow through natural fault zones: The same principles as mentioned above hold here except that, due to the large difference in density, the upward flow of methane continues as long as free-phase methane is present.

M2 Flow through leaky boreholes (well integrity problem): See F1.

M3 Flow through the rock: Some amount of methane which is mobilised during the hydraulic fracturing process may escape from the reservoir through the fractures. This methane would no longer be trapped by adsorption or low permeability and would rise due to buoyancy.

Limitations, general aims and approach of the modelling activities

Hydro-geological systems are heterogeneous by nature. Hydraulic parameters such as porosity and, in particular, permeability can vary strongly in space and in certain cases also in time. A sound knowledge of hydro-geological boundary conditions and the hydraulic parameters are prerequisites for the correct prediction of fluid flow and transport in the subsurface. Typically, these parameters are determined, e.g. by core samples, pumping tests or with numerical models via inverse modelling. The transfer of hydraulic parameters from one location to another is not straightforward, since they can vary strongly even within the same rock type. Hydro-geological simulations can only be considered predictive for a specific location if the parameters are sufficiently supported by field measurements.
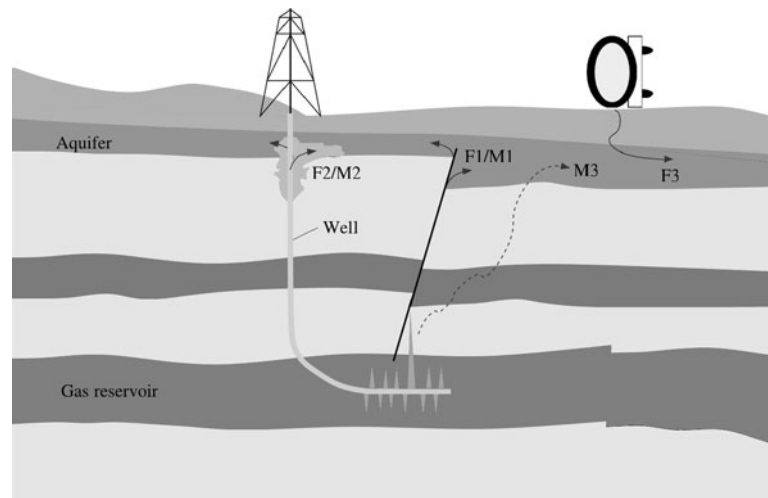
During the hydraulic fracturing process, fractures develop in the gas reservoir, in the shale or in the coal bed. These fractures are typically much more permeable than the background rock. Geo-mechanical modelling tools can be used to predict fracture propagation upon which discrete fracture models or up-scaled, dual-porosity reservoir models can be applied to simulate fluid flow. However, it must be noted that, currently, available modelling capabilities for fracture generation and propagation still rely on strong assumptions. In reservoir engineering, such tools together with measurement data (log interpretations, core analysis, micro-seismic data, etc.) are used for optimising shale gas production (Du et al. 2009). Similar techniques are used in enhanced geothermal systems, where low-permeable reservoirs are stimulated (Tenzer et al. 2010). However, an exact analysis of the hydraulic fracturing process as well as the production and post-production phases with simulations is only possible for a specific test site for which (with the appropriate monitoring) the model can be calibrated and validated. Validation means that the given model can adequately describe the physical processes which occur in the system of interest. This is not considered within the scope of this work. Examples of models for flow in fractured reservoirs that were applied on realistic fracture geometries are presented in Koike et al. (2011) and Tatomir et al. (2011).

The scenarios studied here do not explicitly include the gas reservoir in the model setup. Instead, it is replaced, in a conservative assumption, by a boundary condition for the geological layers which lie above it. The choice of this boundary condition in each of the scenarios is explained in the following sections. No scenarios were set up which describe the flow/leakage paths F2, F3 and M2. These would imply a failure of the operational system. Issues concerning the safety of the operational or technical system are not treated in this work but are part of the working group Risks in Technical Systems (Uth 2012) within the framework of ExxonMobil's hydrofracking dialogue and information dissemination process. A predictive simulation of the transport of fracturing fluid or methane in shallow aquifers is only possible with a site-specific and adequately calibrated groundwater model. To avoid contamination due to such operational accidents, a proper monitoring system with which leaking fluids can readily be detected is necessary. It is also important to be able to simulate the potential spreading of a contaminant plume using groundwater models which may be available for the given site or which are specifically developed for this purpose by the site operator. Such groundwater models are usually available in drinking-water catchment areas. For sites without an adequate groundwater model, the operator should be obliged to set up one during exploration, making use of field data, e.g. from pumping tests. Models like the ones described above can be used to acquire information as to where and when and at what concentration contaminants in an aquifer can be expected, if a failure in the operational system occurs. Possible adverse effects of the chemicals used in fracturing fluids on the environment and human health are assessed in the working group toxicology and groundwater (Riedl et al. 2013; Gordalla et al. 2013).

For more comprehensive risk assessment, the approach used here is not considered suitable. According to a methodology described by Walter et al. (2012), we suggest distinguishing between the specific hazardous scenarios which result in a certain damage and the likelihood of a hazardous event to occur. The combination of damage and likelihood would allow a quantification of risk. However, this requires a much better knowledge of site-specific conditions such as parameter variability, geological structures, etc., than typically available. King (2012) takes an overall look at fracturing risks at different levels (from well construction to production). He defines the identification,

the probability of occurrence and the impact of a hazardous event as a basis for ranking risk. Probabilities for example of a fracture penetrating shallow aquifers are obtained from reported events. The impact is estimated as a certain "worst case" quantity. Myers (2012) takes a different approach (not probabilistic) in a recent numerical study for the Marcellus Shale and states that contaminants from the stimulated reservoir may reach shallow aquifers in less than 10 years through natural vertical flow paths. The study further claims that through the reservoir stimulation, the overall system (shale and overburden) may need 3–6 years to return to pre-injection pressures.

The scenarios developed in this study deal with the flow/leakage paths F1, M1 and M3 as described in the previous section. As a result of the modelling limitations described above (no site-specific field data, no calibration), the scenarios developed here have a predominantly qualitative rather than quantitative value. *Thus, the aim of this study is to determine under which circumstances fracturing fluids or methane in the gas reservoir would leak into shallower layers.* Furthermore, the simulation results can help to illustrate the relevant processes and their relative importance.

The assumptions and simplifications made for each scenario are intended to depict a conservative approach as described by Lange et al. (2013). They are, hence, improbable but still physically possible extreme cases. The work described in this paper aims at documenting the status of our publicly accessible research in Germany on modelling the processes during hydraulic fracturing and subsequent gas production. Presently, the discussion on hydraulic fracturing is rather new for the German society, and the availability of reliable data for modelling is scarce. As stated above, the authors were involved in a dialogue and information dissemination process on hydraulic fracturing in Germany. The authors are also aware that the procedure of the described work does not fulfill all the criteria of the state of the art in the scientific community for modelling flow and transport processes in the subsurface. A number of simplifications were made in the scenarios below, which could be addressed by state-of-the-art methods for building more complex models and with more time. However, more complexity is only justified when the increased demand for reliable data can be met satisfactorily. We do not want to pretend a higher reliability and relevance of our results than that allowed by available data.

Assumptions, scenario setup and results

Three types of scenarios (Scenarios 1, 2, and 3) have been developed which differ with regard to spatial scale, temporal scale, fluid and driving forces. The main differences

in the three scenarios are listed in Table 1. Scenarios 1 and 2 deal with the transport of fracturing fluid and brine in the subsurface. The fracturing fluid is considered to be a conservative tracer in the water phase, which means that processes such as adsorption and biological/chemical degradation which could lead to a gradual reduction in concentration are neglected. Though the viscosity of the fracturing fluid depends on its composition—which can vary strongly—, it is typically larger than that of water. Thus, considering the fracturing fluid as a component in the water phase is a conservative assumption, since the comparatively low viscosity of water leads to higher velocities. This allows the extension of these simulations to account for brine in the same way as for fracturing fluids. Hence, potential trace elements in the brine are treated as conservative tracers. The fluid displaced from the gas reservoir can also be a mixture of fracturing fluid and brine. This approach neglects possible density differences between the injected fracturing fluid (density $\approx 1{,}000$ kg/m^3) and brine (density $>1{,}100$kg/m^3), which lead to buoyancy forces. Scenario 3 deals with the potential migration of methane from the gas reservoir into shallower geological layers.

The results of these three scenarios were previously presented in Sauter et al. (2012) and Kissinger et al. (2012). For all the simulations in this study, the simulation software DuMu^x was used. DuMu^x is an open-source software for the simulation of flow and transport in porous media (Flemisch et al. 2011). The general formulation of the fully coupled multi-component two-phase isothermal mass balance equation used in all of the scenarios is

$$\sum_{\alpha} \frac{\partial \left(\phi S_\alpha \varrho_\alpha X_\alpha^\kappa \right)}{\partial t} = \nabla \cdot \sum_{\alpha} \left\{ \varrho_\alpha X_\alpha^\kappa \frac{k_{\mathrm{rel},\alpha} \mathbf{K}}{\mu_\alpha} (\nabla p_\alpha + \varrho_\alpha \mathbf{g}) \right\}$$
$$+ \nabla \cdot \sum_{\alpha} \left\{ \varrho_\alpha D_{pm,\alpha}^\kappa \nabla X_\alpha^\kappa \right\} + q \qquad (1)$$

where κ stands for the component water, salt, conservative tracer or methane, α stands for either the water phase or the gas phase, ϕ is the porosity, S_α the phase saturation, ϱ_α the phase density, X_α^κ the mass fraction of component κ in phase α, $k_{r,\alpha}$ the relative permeability of the phase, μ_α the phase viscosity, $\mathbf{K}$ the intrinsic permeability tensor, p_α the phase pressure, $\mathbf{g}$ the gravity vector, $D_{pm,\alpha}^\kappa$ the diffusion coefficient of the porous medium and q is a source or sink term. For the temporal discretisation, the fully implicit backward Euler method is used; hence there is no stability-motivated time–step size constraint. The BOX method, which is a node-centered finite-volume method based on a finite-element grid is used for spatial discretisation. For more information on the temporal and spatial discretisation and solution concepts used here, the authors refer to Helmig (1997). The constitutive parameters used in solving the mass balance equations are given in Table 2. A static

temperature gradient of 30 K/km is assumed in all the scenarios to account for changes in density and viscosity. Therefore, the strong decrease in methane density which occurs during an upward migration (related more to changes in pressure than in temperature) can be reproduced by this model. However, no energy balance is included in the system of equations as energy transport is considered to have a negligible effect on the processes described here. Furthermore, mechanical dispersion is neglected in all scenarios, since there is no available field data to calibrate the model. Mechanical dispersion would lead to smaller concentrations and a larger areal spread of the contaminant plume. Numerical dispersion, which is a result of spatial and temporal discretisation lengths, as well as the fully upwind scheme applied in this model has similar effects which are however hard to quantify.

Assumptions and setup of Scenario 1

Assumptions for Scenario 1: In Scenario 1 the potential transport of fracturing fluids, which escape from the gas

reservoir, in both shallow and deep aquifers is in the focus of interest. The driving forces of flow are the strong vertical pressure gradients, which develop due to the hydraulic fracturing operations. As described above, the gas reservoir is not simulated explicitly, but accounted for as a boundary condition. The increase in pressure at the interface between the gas reservoir and the overburden due to hydraulic fracturing is varied. These pressures, which are superimposed on the hydrostatic pressure, are set as boundary conditions. The schematic setup of the scenario is shown in Fig. 2. The pressure evolution (boundary condition) at the boundary between the gas reservoir and the overburden is shown in Fig. 3.

In the simulations, this pressure is applied either directly at a fault zone or in the intact overburden. Scenario 1 is simulated for the seven settings described in Lange et al. (2013) including their various parameters such as aquifer thicknesses, porosity and permeability. The assumption that the pressure induced by hydraulic fracturing is valid at the interface between the gas reservoir and the overburden is a very conservative one, since it implies that the fractures created during hydraulic fracturing operations spread all the way to the overburden. Furthermore, no reduction in pressure between the borehole (at which the maximum pressure prevails) and the overburden takes place which is obviously not realistic. The maximum pressure is taken to be constant for a period of 2 h. In reality, however, one would expect a drop in pressure if the fracturing fluid penetrates a permeable fault zone.

The assumptions made for this scenario are schematically summarised in Fig. 4. The target dependent variable in Scenario 1 is the vertical extent of the fracturing fluid or brine. It depicts qualitatively the distance over which a potential contaminant could spread under these unfavourable conditions as explained above.

Table 1 Scenario properties

	Scenario 1	Scenario 2	Scenario 3
Spatial scale	Local	Regional	Local
Temporal scale	Short term	Long term (30 years)	Long term (100 years)
Fluid	Fracturing fluid and brine	Fracturing fluid and brine	Methane
Driving force	Pressure gradient due to fracturing	Natural horizontal and vertical pressure gradient	Gravitation and capillary forces

Table 2 List of constitutive relationships and their sources

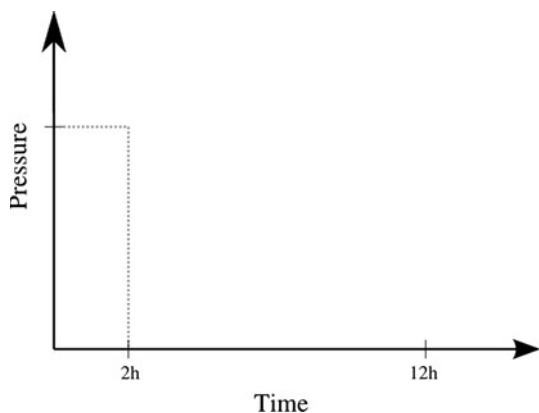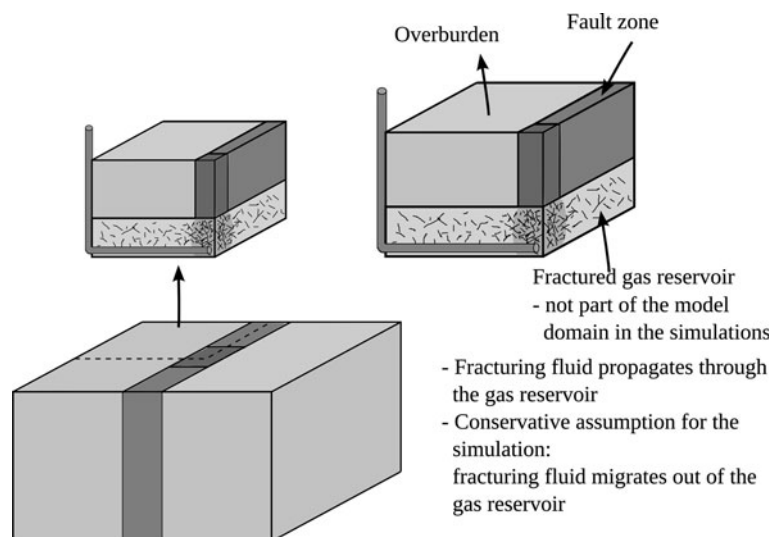| Parameter	Unit	Function of…	Source
Brine density	kg/m^3	Pressure, temperature and salinity	Batzle and Wang (1992)
Methane density	kg/m^3	Pressure and temperature	Ideal gas
Brine viscosity	kg/(ms)	Temperature and salinity	Batzle and Wang (1992)
Methane viscosity	kg/(ms)	Temperature	Reid et al. (1988)
Solubility of methane in brine	kg: CH$_4$/kg brine phase	Pressure, temperature and salinity	Duan et al. (1992a, b)
Vapour content in gas phase	kg H$_2$O/kg gas phase	Pressure, temperature and salinity	Duan et al. (1992a, b)
Relative permeability of brine	–	Brine saturation	Brooks and Corey (1964)
Relative permeability of gas phase	–	Gas saturation	Brooks and Corey (1964)
Capillary pressure	Pa	Brine saturation	Brooks and Corey (1964)
Diffusion coefficient of conservative tracer in gas phase	m^2/s	Constant 1.0×10^{-9}	
Diffusion coefficient of methane in brine phase	m^2/s	Pressure and temperature	Reid et al. (1988)
Diffusion coefficient of water in gas phase	m^2/s	Pressure and temperature	Fuller et al. (1966)

Fig. 3 Qualitative evolution of the pressure conditions at the interface between the gas reservoir and the overburden

Setup of Scenario 1: The simulations of Scenario 1 were performed with a one-phase (i.e. water), three-component (i.e. water, salt and a conservative tracer) model. The salinity increases with depth up to a maximum value of 0.1 kg NaCl/kg brine. The tracer can represent any of the components from the gas reservoir (i.e. fracturing fluids or brine). The density of the water phase is a function of salinity as well as of pressure and temperature. Owing to symmetry, only a quarter of the total model domain is simulated. The various simulations are parametrised to fit the seven hydro-geological settings as described by Lange et al. (2013). The parametrisation of the hydro-geological settings is given in detail in Online Resource 1. For Lower Saxony, values from literature were used to characterise the fault zones (see Lange et al. 2013). The width of the fault (damaged) zone is set at 30 m as shown in Fig. 5. An area of leakage of 100 m x 30 m is chosen and located directly under the overburden. At the above-mentioned leakage area (shown in Figs. 2, 5), a constant-head boundary

condition is set to a value that is equivalent to the hydraulic head required for fracturing. Simultaneously, the tracer concentration and the salinity of the water phase are constant over this area. An overpressure (compared to the initial hydrostatic pressure), which ranges from 50 to 700 bar (a plausible range for hydraulic fracturing operations) is assumed. The individual simulations have different maximum pressures, as the pressure needed to stimulate a reservoir increases with depth due to increasing stress magnitudes. A total time of 12 h is simulated, of which 2 h constitutes the actual fracturing time (high pressure). The remaining 10-h interval is a relaxation period. The parameters which are varied for the different settings are shown in Table 3. In Scenario 1 each setting is split into two cases:

– Reference case without fault zone.
– Fault zone as parametrised in Table 3.

Initially, hydrostatic pressure is assumed. The setup and some results of a simulation for the location Borken are shown in Fig. 6. The grid used for the setting Lünne is shown in Fig. 7 and is representative of the other simulations as well.

Results and discussion of Scenario 1

The results for the nine simulations of the setting Bad Laer are given in Table 4 and Fig. 8. The results show that a limited vertical transport distance of 50 m is possible if the permeability of the fault zone is 10^{-13} m^2 (see Simulation 9 in Table 4). The threshold for detecting the maximal vertical migration length is a tracer concentration reduced by a factor of 100 compared to the initial tracer concentration. The second largest transport distance of about 20 m

Fig. 4 Illustrative representation of the conservative assumptions made in Scenario 1 (shown here for the Münsterland Basin as an example)
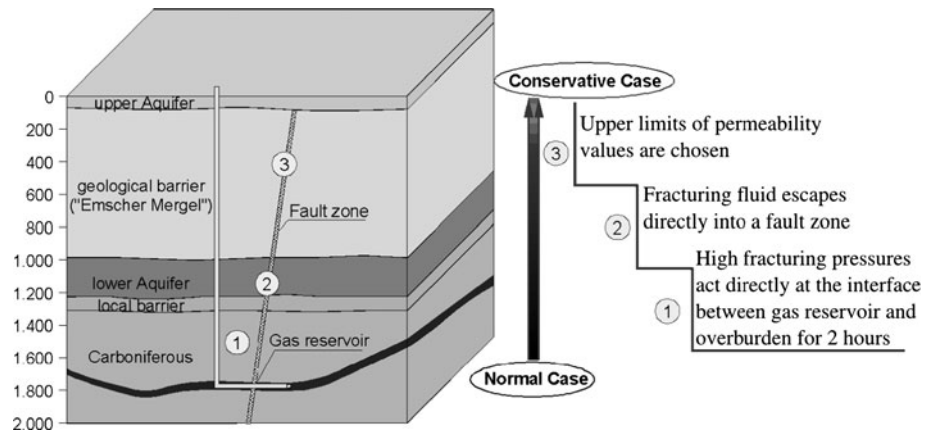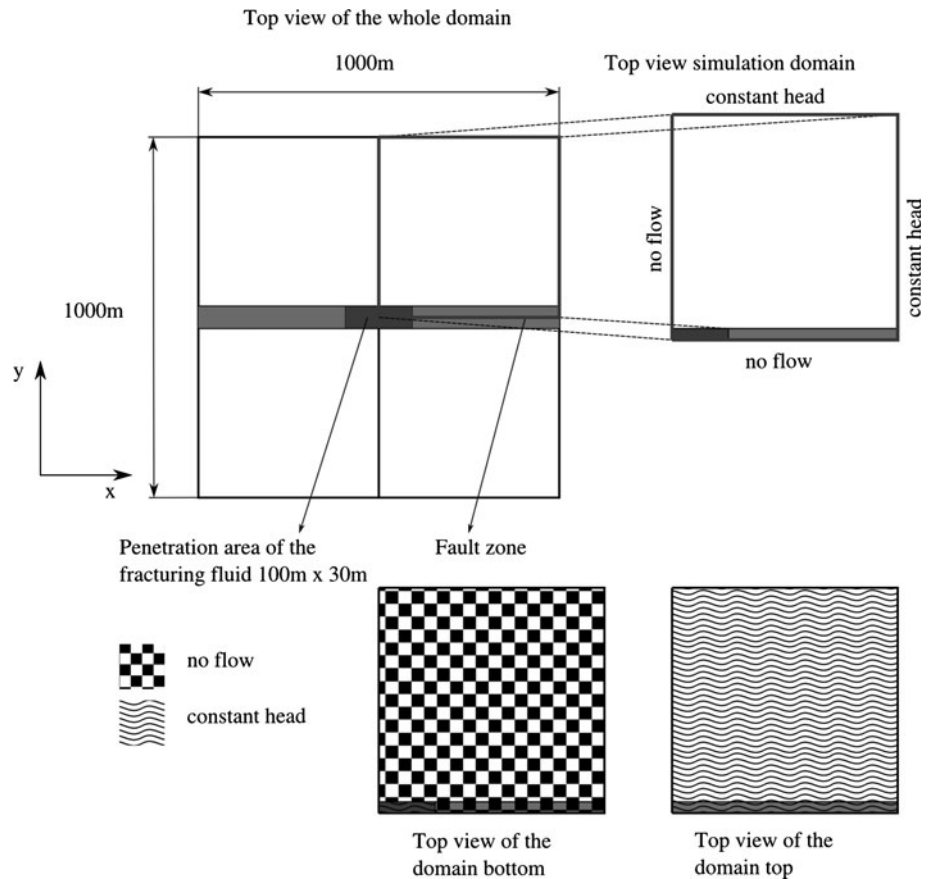

Fig. 5 *Top view* of the model domain and the simulation domain (one-quarter of the model domain) and the boundary conditions set at the side planes as well as on the *top* and *bottom* planes

is reached in the setting Borken (Permeability: 1×10^{-14} m²), also for the upper limit of the parameter combination (see Table 3). For the settings in Lower Saxony (Lünne, Damme, Quakenbrück-Ortland and Vechta), no significant spreading of the fracturing fluids takes place, even at an overpressure of 700 bar (Quakenbrück-Ortland and Vechta) over 2 h. This is mostly due to the low permeability assumed for the fault zones in Lower Saxony (1×10^{-16} m²).

For the reference cases without a fault zone where the large overpressures act directly at the overburden, no

significant spreading is observed. Hence, the transport of fracturing fluid or brine depends primarily on the hydraulic parametrisation of the fault zone. For more detailed results of all the settings, the authors refer to the final report of the group "Risks in the Geological System" (Sauter et al. 2012).

The simulation results show that a limited vertical spreading (maximum is 50 m in setting Bad Laer) is possible if the fault zone has a high conductivity. The assumption of a constant pressure of up to 300 bar right at the fault zone for a period of 2 h is extremely conservative.

Table 3 Upper and lower limits of the parameter combinations used in the simulations

Setting	Upper limit			Lower limit		
	Permeability (m^2)	Porosity (−)	Overpressure (bar)	Permeability (m^2)	Porosity (−)	Overpressure (bar)
Borken	1.8×10^{-14}	0.01	300	1.7×10^{-17}	0.001	50
Bad Laer	9.0×10^{-14}	0.01	300	2.6×10^{-16}	0.001	50
Nordwalde	5.9×10^{-15}	0.01	300	2.4×10^{-17}	0.001	50
Lünne	1.0×10^{-16}	0.01	300	1.0×10^{-17}	0.001	50
Damme	1.0×10^{-16}	0.01	300	1.0×10^{-17}	0.001	50
Quackenbrück	1.0×10^{-16}	0.01	700	1.0×10^{-17}	0.001	150
Vechta	1.0×10^{-16}	0.01	700	1.0×10^{-17}	0.001	150

Fig. 6 *Left* model setup for Scenario 1. *Right* simulation result for the setting Borken
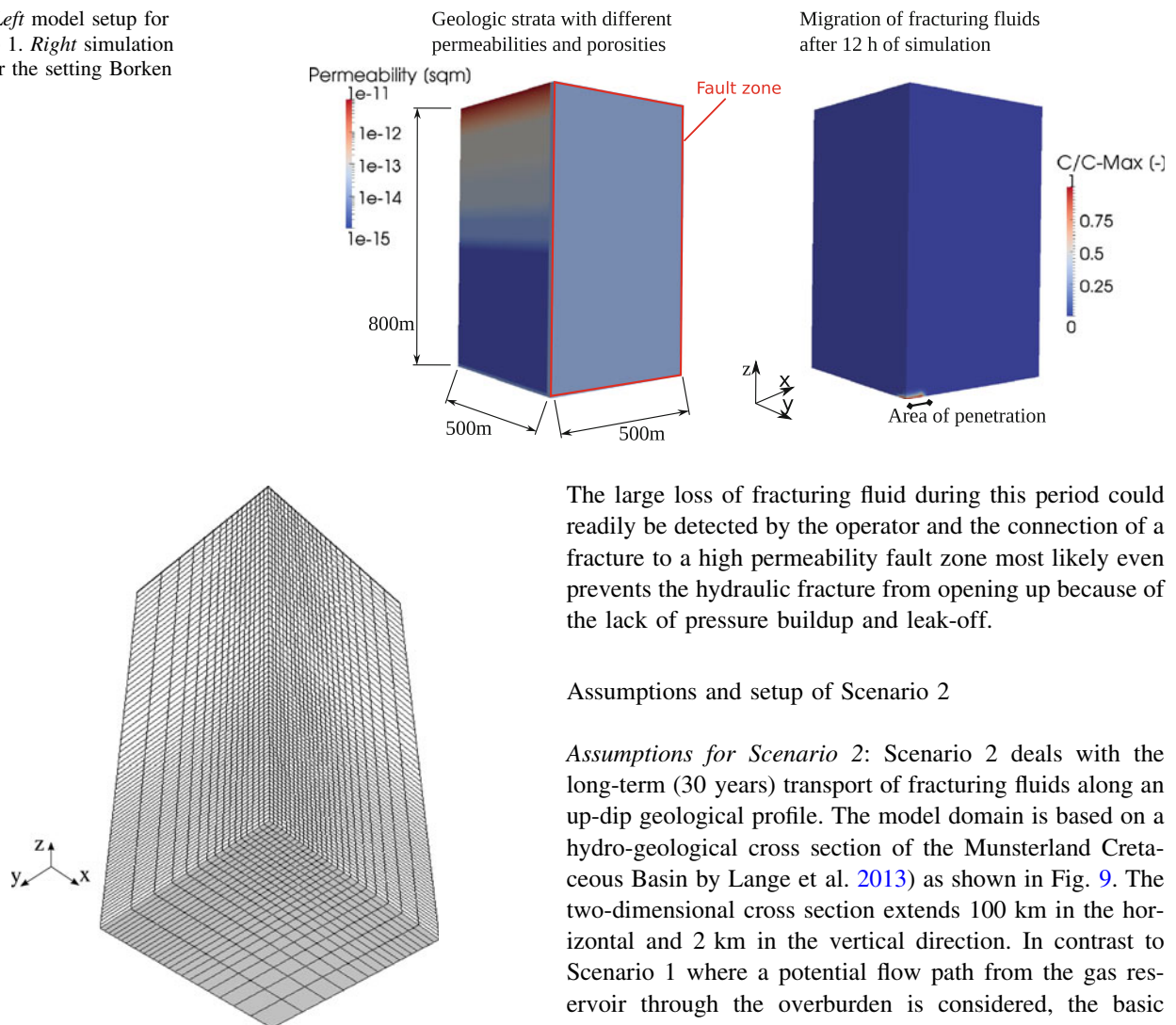

Fig. 7 The grid used in the simulation for the setting Lünne for Scenarios 1 and 3 (view from the *bottom* of reservoir to the *top*). The hexhedron grid is refined close to the penetration area of the fracturing fluid or methane and the cell size decreases logarithmically towards the outer boundaries. The cell size varies from 10 and 100 m. Grids of similar type were also used for all the other settings

The large loss of fracturing fluid during this period could readily be detected by the operator and the connection of a fracture to a high permeability fault zone most likely even prevents the hydraulic fracture from opening up because of the lack of pressure buildup and leak-off.

Assumptions and setup of Scenario 2

Assumptions for Scenario 2: Scenario 2 deals with the long-term (30 years) transport of fracturing fluids along an up-dip geological profile. The model domain is based on a hydro-geological cross section of the Munsterland Cretaceous Basin by Lange et al. 2013) as shown in Fig. 9. The two-dimensional cross section extends 100 km in the horizontal and 2 km in the vertical direction. In contrast to Scenario 1 where a potential flow path from the gas reservoir through the overburden is considered, the basic assumption in Scenario 2 is that a given amount of fracturing fluid has already leaked into the deep Cenomanian–Turonian aquifer system.

The assumption (previously explained) that the fracturing fluid is a conservative tracer (no degradation, no adsorption) leads, in the long run, to a strong overesti-

Table 4 Results of the nine simulations for the setting Bad Laer

Simulation	Overpressure (bar)	Permeability of fault zone (m^2)	Porosity of fault zone (−)	Width of the fault zone (m)	Vertical transport distance (m)
1	50	–	–	–	0
2	50	2.6×10^{-16}	0.001	30	0
3	50	9.0×10^{-14}	0.01	30	0
4	150	–	–	–	5
5	150	2.6×10^{-16}	0.001	30	5
6	150	9.0×10^{-14}	0.01	30	29
7	300	–	–	–	12
8	300	2.6×10^{-16}	0.001	30	12
9	300	9.0×10^{-14}	0.01	30	48
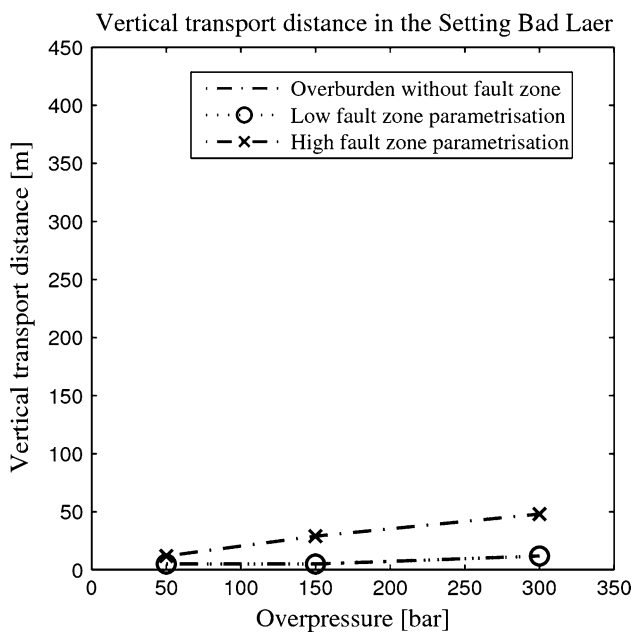
Fig. 8 Results of Scenario 1 for the setting Bad Laer. The nine simulations in the figure correspond to the simulations in Table 4 where high and low fault zone parametrisation refers to a high or low permeability of the fault zone. The *bottom* of the model domain is 450 m below the ground surface level

mation of the concentrations. The saline groundwater in the deep aquifer system has a higher density than the groundwater in the shallow freshwater aquifer. Thus, an upward movement of the saline water is only possible if the hydraulic head in the Cenomanian–Turonian is higher than in the shallower layers, i.e. if it is an artesian aquifer. The Münsterland Basin does have artesian aquifers (Lange et al. 2013). If a fault zone of high permeability penetrates such an artesian aquifer, this can lead to an upward flow of deep saline water due to the vertical hydraulic-head gradient. As such, this mechanism could lead to the upward transport of fracturing fluids.

The conservative assumptions made for Scenario 2 are summarised in Fig. 10. The aim here is to determine whether these conservative but still plausible conditions can lead to a significant migration of fracturing fluids through a fault zone. To this end, permeability and porosity distributions as well as the potential leakage path have to be chosen.

Setup of Scenario 2: The simulations of Scenario 2 were performed with a single-phase (i.e. brine), two-component (i.e. brine and a conservative tracer) model. The salinity is treated as a pseudo-component, i.e. there is a given vertical salinity gradient which, however, remains constant throughout the simulations. As in Scenario 1, the maximum salinity (at the bottom of the domain) is 0.1 kg NaCl/kg brine. The two-dimensional model domain is shown in the cross section in Fig. 9. An unstructured triangular mesh refined in the area surrounding the fault zone was set up for this purpose. The simulation time is 30 years. The model setup includes a fault zone as can be seen in the figure. It also accounts for the geological layers. The parameters used to describe these layers and the fault zone are listed in Table 5. The domain is bounded at the bottom by carboniferous bedrocks, which are assumed to be a no-flow boundary. The hydraulic head at the top boundary is considered to be constant. It is slightly lower in the Quaternary corresponding to the presumed vertical gradient. The distribution of the hydraulic head as well as the allocation of the boundary conditions is shown in Fig. 9. The global, ambient pressure gradient (horizontal) is 4.4×10^{-4}. Initially, a contaminant plume of dimension 100 m x 100 m is assumed to be present in the Cenomanian–Turonian aquifer. Table 6 gives an overview of the simulations, including the range of variation of the vertical hydraulic-head (piezometric) difference between the Cenomanian–Turonian and Quarternary aquifer. The parametrisation of the different layers and the fault zone as well as the determination of the horizontal and vertical gradients is explained in more detail in Lange et al. (2013).

Fig. 9 A potential fault zone (as used in this simulation) penetrates the Münsterland Basin. Also shown are the boundary conditions used in this model setup and the unstructured *trinangular* grid
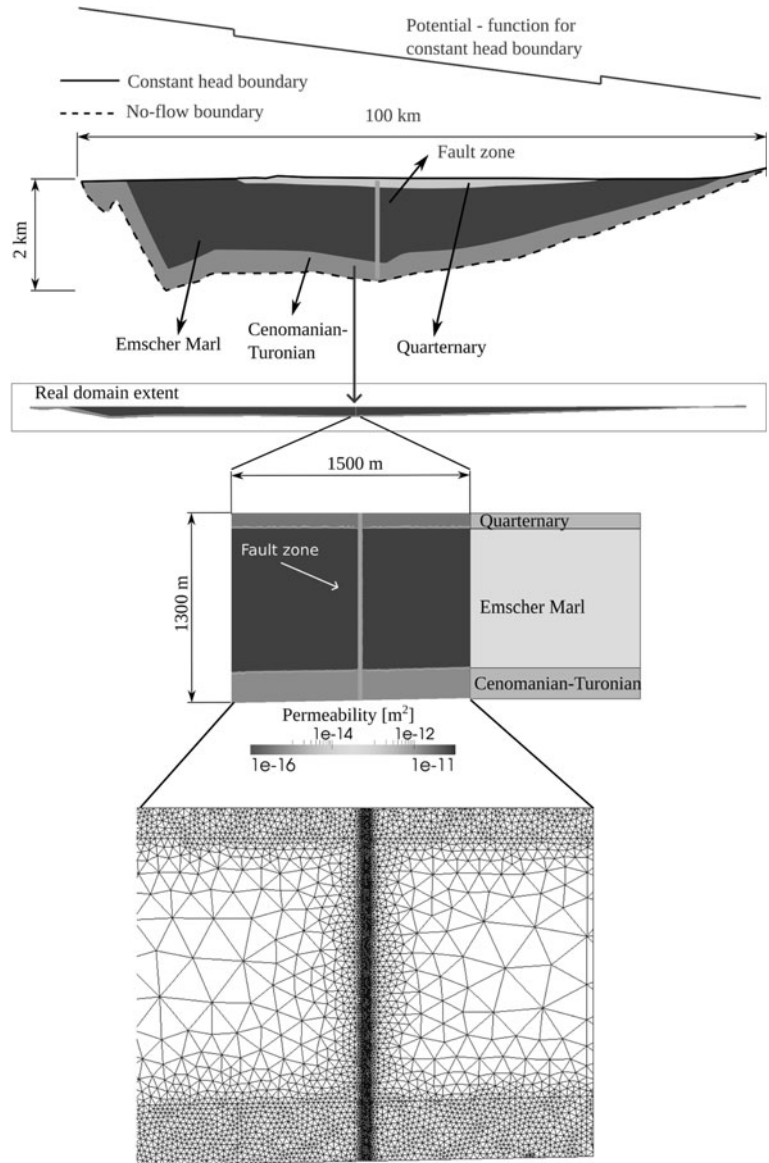

Fig. 10 Illustrative representation of the conservative assumptions made in Scenario 2 (shown here for the Münsterland Basin as an example)
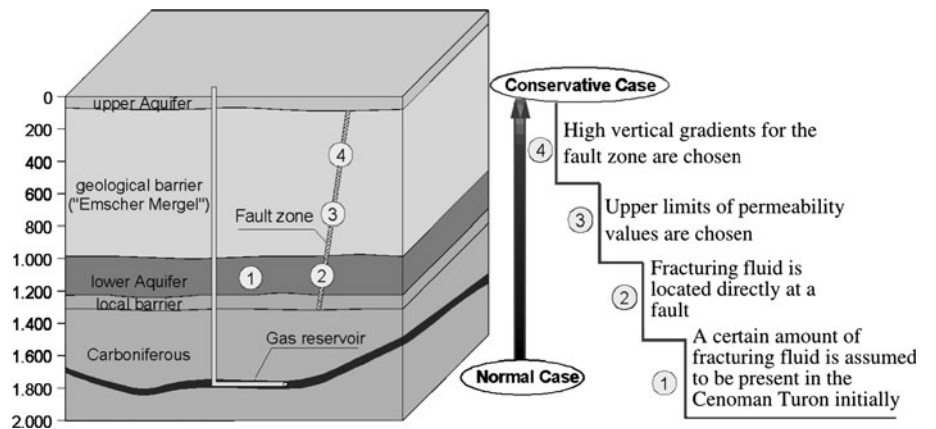
Table 5 Parametrisation of the geological strata in Scenario 2

Formation	Permeability (m^2)	Porosity (−)
Cenomanian/Turonian	3×10^{-13}	0.01
Emscher marl	1×10^{-18}	0.001
Quarternary	1×10^{-12}	0.1

Table 6 Variation of the hydraulic-head gradient and the fault zone permeability

Simulation	Fault zone permeability (m^2)	Fault zone porosity (−)	Hydraulic head difference (m)
1	1×10^{-13}	0.01	0
2	1×10^{-13}	0.01	30
3	1×10^{-13}	0.01	60
4	1×10^{-15}	0.01	30
5	1×10^{-15}	0.01	60

Results and discussion of Scenario 2

The results of Simulations 1 and 3 are shown in Figs. 11 and 12. In Simulation 1 (see Fig. 11), for which the vertical head gradient is zero, one can see that there is no vertical transport along the fault zone. The contaminant spreads in the permeable Cenomanian–Turonian aquifer as a result of the ambient hydraulic gradient, which prevails in the Münsterländer Basin. Since degradation, sorption processes and mechanical dispersion are neglected, it must be noted that the concentrations in the simulations are higher than one would actually expect. For high values of the vertical hydraulic-head difference [60 m in Simulation 3 (see Fig. 12)], the vertical transport within the fault zone leads to fracturing fluid or brine reaching the Quarternary with a concentration reduced by a factor of 4000 due to mixing processes (and by numerical diffusion—not quantified here) with respect to the initial concentration of the conservative tracer. There is no vertical transport in the Emscher Mergel as a result of its low permeability (see Table 5, 1×10^{-18} m^2). In Simulations 4 and 5, there is no transport through the fault zone as its permeability is reduced by two orders of magnitude (see Table 6, 1×10^{-15} m^2). This shows that the transport processes are strongly dominated by the ratios between the permeabilities of the Cenomanian–Turonian aquifer (3×10^{-13} m^2) and the fault zone (1×10^{-13} m^2) as well as between the horizontal and vertical head gradients. The results for all five simulations are given in the final report of the working group "Risks in the Geological System" (Sauter et al. 2012). In summary, the vertical transport of the fracturing fluid in the Cenomanian–Turonian aquifer to shallower strata through the fault zone is possible only for the most conservative simulation (Simulation 3). However, the concentration is strongly reduced when compared with the initial tracer concentration (factor 4000). The simulated scenario is conservative (only the fault zones with a high permeability in the range of 1×10^{-13} m^2 show migration) but plausible for the Münsterländ Basin. However, it presumes that fracturing fluids or brine can escape from the gas reservoir into the Cenomanian–Turonian aquifer, which is considered an unlikely event (see Scenario 1). Inferences concerning the danger this could pose for a freshwater aquifer can only be made with a more detailed and site-specific investigation. General statements in this regard are not possible here.

Assumptions and setup of Scenario 3

Assumptions for Scenario 3: Scenario 3 deals with the long-term transport (100 years) of methane from the gas

Fig. 11 Simulation 1—The figure shows the spreading of a contaminant in the Cenomanian–Turonian aquifer and in the fault zone. The values of the concentration are normalised with respect to the initial concentration of the conservative tracer. The *left figure* shows the initial state of the plume, while the *right figure* shows the spreading of the plume after 30 years. The vertical hydraulic head gradient is zero. The area shown corresponds to the extract of the whole domain in Fig. 9
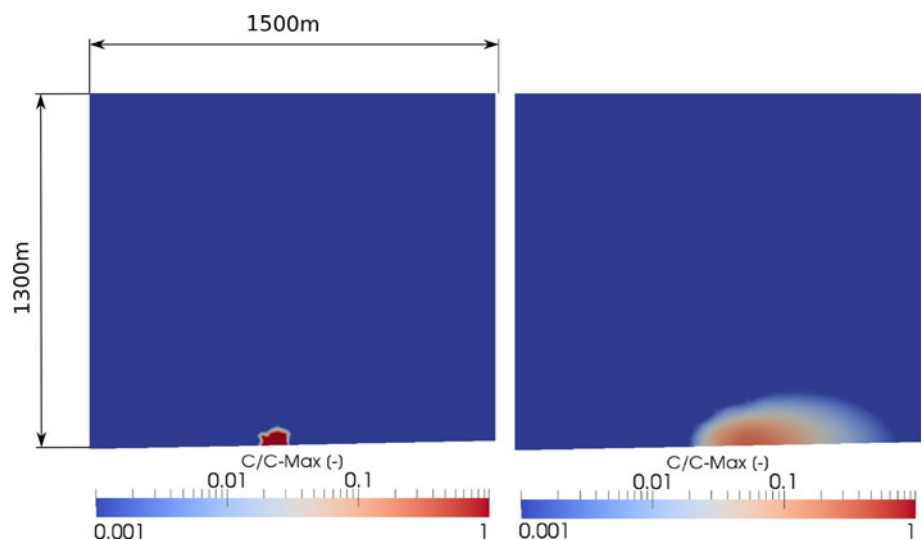
Fig. 12 Simulation 3—The *figure* shows the spreading of a contaminant in the Cenomanian–Turonian aquifer and in the fault zone. The values of the concentration are normalised with respect to the initial concentration of the conservative tracer. The *left figure* shows the initial state of the plume, while the *right figure* shows the spreading of the plume after 30 years. The vertical hydraulic head gradient is equal to 60. The area shown corresponds to the extract of the whole domain in Fig. 9
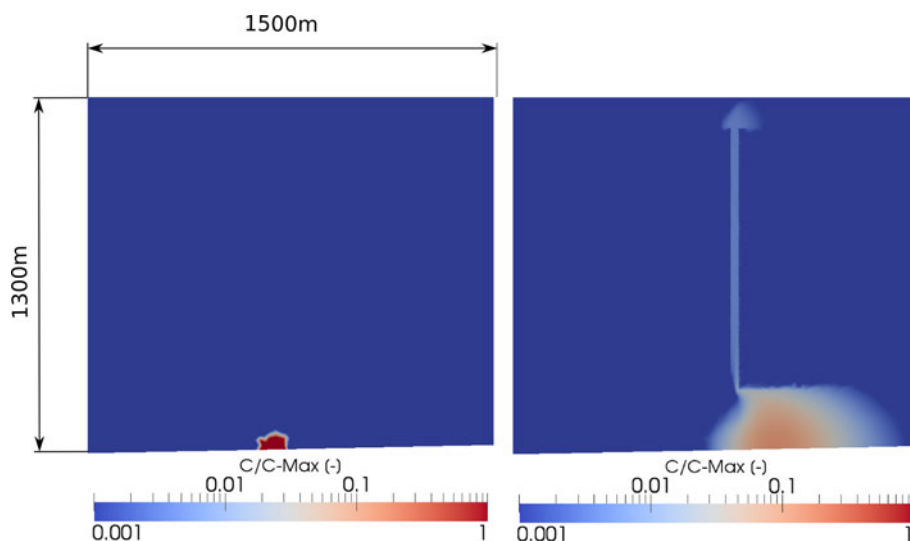
Fig. 13 Schematic setup of the model domain for Scenario 3
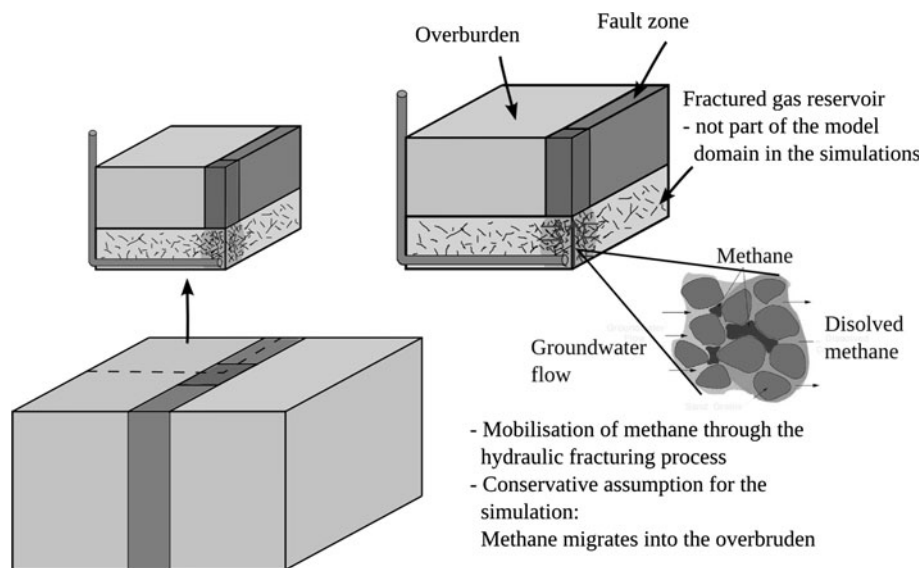
reservoir through the overburden. The driving force here is buoyancy due to the density difference between the gaseous (and thus very light) methane and the water phase. In addition, capillary forces which differ from layer to layer cause a lateral spreading of methane.

As is the case for the other scenarios, the gas reservoir is not considered here, since it would entail a very complex geological model which also accounts for the fractures in the reservoir. The model setup is to a large extent analogous to Scenario 1 as apparent from Fig. 13.

A constant flux of methane across the boundary between the gas reservoir and the overburden is chosen as the boundary condition. The value of this flux is explained in the model setup below. It is worth noting, however, that the assumption of a constant flux across the boundary is very

conservative. A constant escape of gas from the reservoir is rather improbable.

Hydro-geological settings of shale and tight gas sites (Lünne and Vechta) in Lower Saxony (Lange et al. 2013) are simulated here. The parametrisation of these hydro-geological settings is given in detail in Online Resource 1.

One of the most important parameters which determines the fate of the methane is the residual gas saturation. Some of the methane that flows through the pore space is immobilised due to capillary effects. This effect is referred to as residual trapping. The volume fraction of immobilised gas is called residual gas saturation (Helmig 1997). For methane, it can vary strongly depending on the type of rock. Other important factors include

Fig. 14 Illustrative representation of the conservative assumptions made in Scenario 3 (shown here for the Münsterland Basin as an example)
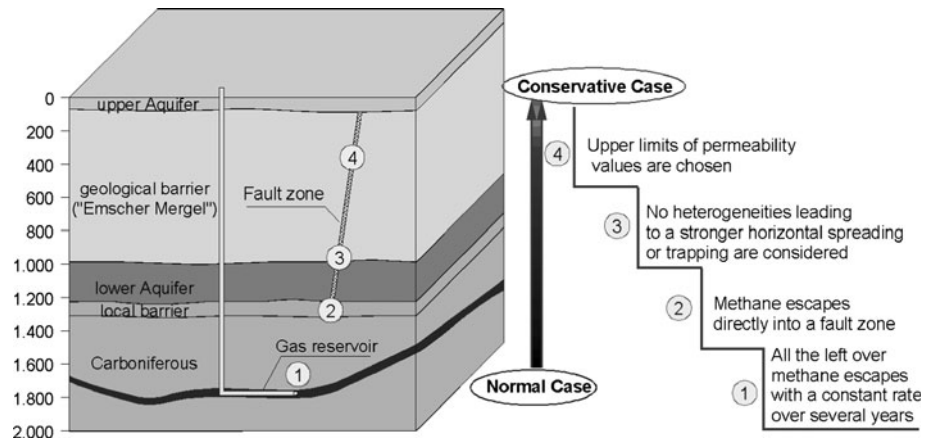

Fig. 15 The density and viscosity of methane over depth are shown for a depth from 0 to 4,000 m below sea level, assuming a geothermal gradient of 30° per 1,000 m with a surface temperature of 10° C and hydrostatic pressure. The density is calculated using the ideal gas law and a more complex non-linear equation of state according to Duan et al. (1992a, b). The viscosity is calculated with a relation by Reid et al. (1988) and Daubert and Danner (1989)
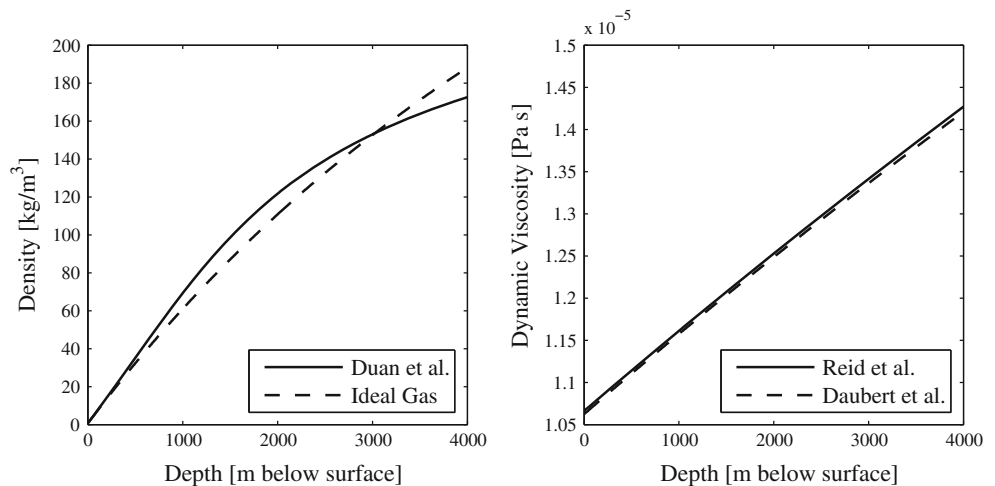
– Heterogeneities (variations of the rock properties such as permeability, porosity, capillary pressure–saturation relationship, relative permeability–saturation relationship, residual gas and water saturations) have a very strong effect on the flow behaviour of methane
– Geological relief of the subsurface strata (e.g. anticlines)

Variations in the geological relief (e.g. sloping aquifers) are, however, not included in this setup. The fault zone is parametrised homogeneously as is the case in Scenario 1. The main assumptions made for this scenario are summarised in Fig. 14.

The large uncertainty in the determination of the boundary condition and the hydraulic parameters of the settings imply that the results of these simulations can be interpreted only qualitatively. Two cases are examined here:

– The fault zone penetrates the full thickness of the overburden
– The fault zone has a reduced permeability when it penetrates the Halite Strata

In addition, the residual saturation of methane is varied in order to demonstrate the large influence of this parameter.

Setup of Scenario 3: The simulations of Scenario 3 were performed with a two-phase (i.e. brine and gas), two-component (i.e. brine and methane) model (Flemisch et al. 2011). In this model, methane can exist as a separate gas phase (with a limited amount of evaporated water) or dissolved in the brine phase. The salinity is assumed to be constant in the whole domain (0.1 kg NaCl/kg brine). The salinity affects the properties of the brine phase and the solubility of methane in the brine phase. The density of gaseous methane varies strongly with increasing depth (i.e. increasing pressure and temperature) as shown in Fig. 15, while the increase in viscosity is more moderate. In the simulations, methane is assumed to behave as an ideal gas. The relatively small deviations from the more complex and computationally demanding equation of state for methane density by Duan et al. (1992a, b) justify this assumption, see Fig. 15. Capillary pressure and relative permeabilities are calculated as a function of saturation using a Brooks and Corey (1964) relationship. Due to lack of data for the Brooks and Corey equations ($\lambda = 3.5$ and $P_e = 1,800$ Pa)

Fig. 16 *Top view* of the model domain and the simulation domain (one-quarter of the model domain). The boundary conditions set at the side planes as well as the *top* and *bottom* planes are also shown
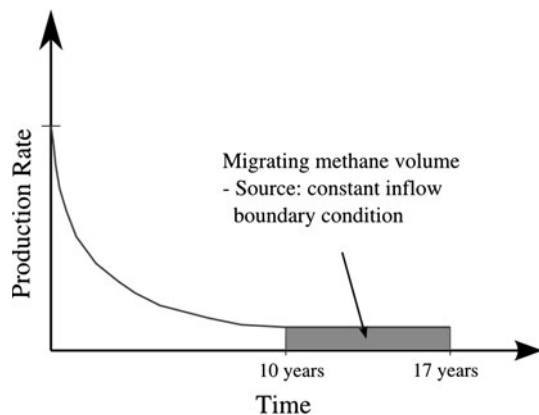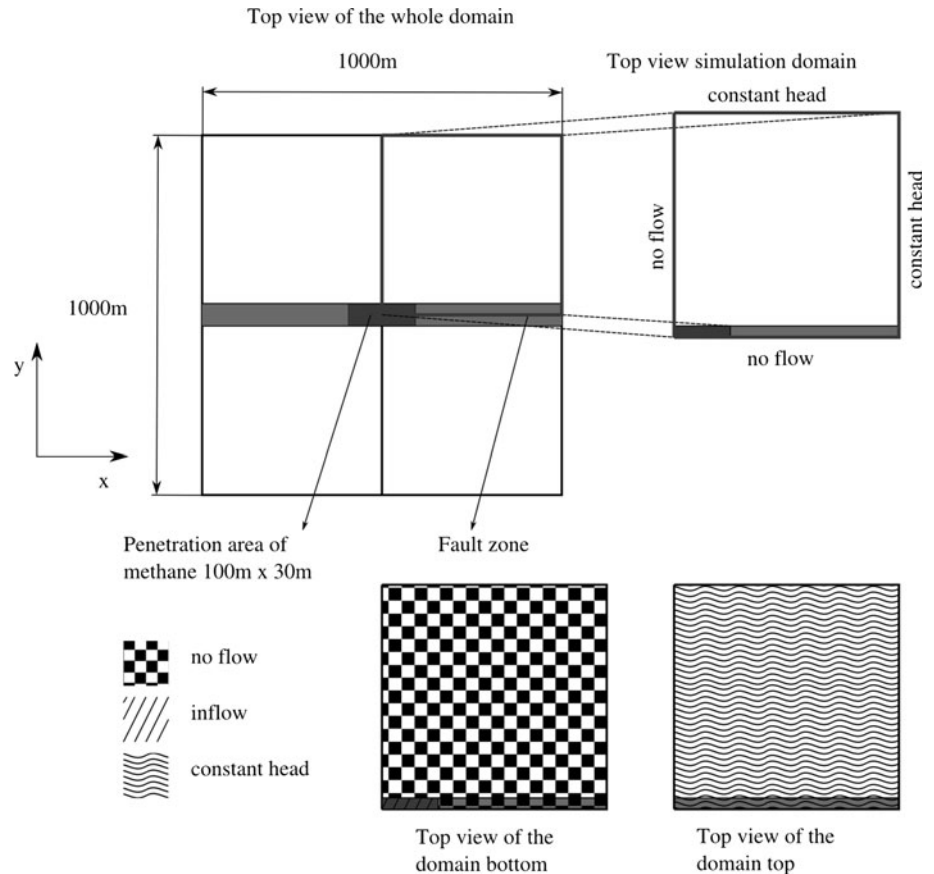

Fig. 17 Example of a methane production curve from a fracturing borehole. The volume of methane which is assumed to leak into the model domain corresponds to the interval between 10 and 18 years. The flux is constant in this area

in the different geological strata, the Leverett J-Function is used to scale these parameters with the ratio of permeability and porosity for the specific layers:

$$J(S_w) = p_c(S_w)\sqrt{k/\phi} \qquad (2)$$

Here, S_w is the water saturation, p_c the capillary pressure, k the permeability and ϕ the porosity. For the residual gas

saturation, no data are available. It is hence varied between 1 and 30 % for the different simulations, which is assumed to cover the range of maximum and minimum values for the various rock types as determined analogously for the brine–CO_2 system (Bachu and Bennion 2007). In addition, the residual gas saturations of different rock types in Nordrhein-Westfalen were included in this estimation (Kunz 1994). The residual water saturation is varied between 18 and 60 %. For low-permeable porous media with a low porosity, residual gas and water saturations are likely to be higher than 1 and 18 %, respectively, as considered in some of the simulations. However, these simulations are still presented here as extreme cases to show the significance of these uncertain parameters on methane migration through the overburden. In the following, the residual saturations are assumed to be the same in all the geological strata. The simulation time for all settings is 100 years. The geometric setup of the model corresponds to that of Scenario 1 with the exception of the fault zone which, depending on the simulation, either has a homogeneous permeability or a partially reduced permeability in the halite strata layers. The top view of the model domain and the simulation domain (analogous to that of Scenario 1) is shown in Fig. 16. The grid used is similar to that of Scenario 1 (see Fig. 7). As mentioned previously, the

methane flux from the gas reservoir into the model domain is a critical quantity. Assumptions in this regard have been made, which of course are questionable. However, at this point it should be noted again that the gas reservoir is included through conservative boundary conditions, which in this case lead to a certain (conservative) methane flux into the overburden. The focus of these simulations lies more on the question of what happens to the methane while it migrates upwards, rather than on the processes taking place in the gas reservoir. In the following, the individual steps taken in determining the flux of methane escaping from the gas reservoir are presented. To this end, the methane volume is required:

– Conservative assumption: production stops after 10 years with no leakage up to this point since flow is directed towards the borehole (pressure gradient towards borehole exceeds buoyancy effects).
– A fraction of the methane left in place after 10 years of production estimated from a typical production curve (see Fig. 17) from the Haynesville Shale in the USA (U.S. Energy Information Administration 2011).
– About 20 % remains in the gas reservoir.
– To obtain the methane flux for one fracturing procedure 20 % of the expected production rate (provided by ExxonMobil) is divided by the number of fracturing procedures per horzontal well.

To determine the rate at which the given volume of methane escapes into the overburden (i.e. flux), the following assumptions are made:

– Estimation of the methane flux based on the production curves after 10 years of production; see Fig. 17.
– Flux is divided by the number of fracs (i.e. the number of hydraulic fracturing operations per horizontal well) to obtain a flux per frac.
– The time over which methane escapes is calculated as → Volume per frac/flux per frac.

In Table 7, the calculation of the flux is summarised and values are provided. Two locations, Haynesville Shale and Eagleford Shale, in the USA are considered, though only the values of the Haynesville Shale are used in the simulation. Initially, hydrostatic pressure is assumed. Table 8 gives an overview of the simulations and the varied parameters.

Results and discussion of Scenario 3

The results of the simulations are summarised in Fig. 19. The value of interest here is the amount of methane that migrates into the shallow Quarternary groundwater system. A migration only occurs in Simulations 1 and 5.

Figure 18 shows the methane saturation in the simulation domain for Simulations 1, 2 and 3. The effect of the varied parameters on the methane migration is illustrated here. In Simulation 1 (Setting Lünne), approximately 20 % by mass of methane which entered the simulation domain could migrate into the shallow groundwater system. In Simulation 6 where the residual water saturation is increased the amount of migrated methane increases to over 60 % (see Fig. 19) and the time until the methane reaches the shallow groundwater system is reduced. This is due to the reduction of pore space caused by the higher residual water saturation. The saturations within the overburden after 100 years in Simulation 1 are higher than in Simulation 6 since the mobility (ratio of relative permeability and dynamic viscosity) observed at this point in time in both simulations is equally low at different saturations. This corresponds well to the slow increase in the migrating mass seen in Fig. 19 towards the end of the simulations. Using the same fault-zone properties and residual saturation for the setting Vechta (Simulation 5), no leakage of methane into the atmosphere is observed. This is a result of the larger overall storage capacity of the different geological layers as well as the fault zone due to the increased depth of the reservoir at this location (3800 m).

A comparison of Simulations 1 and 2 (Fig 18c, d) shows that the residual gas saturation plays a significant role for the migration of methane. In Simulation 1, methane reaches the top boundary, while it only covers a third of the overburden in Simulation 2.

Comparison of Simulation 1 with Simulation 3 (Fig. 18 b, c) shows that at the beginning of the halite strata, there is an increased lateral spreading of methane since the leakage path is blocked. Capillary forces, which differ from layer to layer, are largely responsible for the lateral spreading of the plume. Large amounts of methane leave the domain over the lateral boundaries.

Thus, the simulations show that the leakage of methane into the shallow layers through the overburden is only possible if several assumptions, which we consider conservative are made as is the case in Simulation 1:

– Permeable fault zone
– Low residual saturation and low porosity
– Large volumes of methane mobilised from the gas reservoir
– Shallow gas reservoir (e.g. Lünne 1,200 m)

It must be stated that such a scenario is highly unlikely since no fracturing operations should be carried out in a reservoir with a fault zone that penetrates the full thickness of the overburden. Additionally as mentioned before, a residual gas saturation of 1 % for the whole overburden is an extreme assumption.

Table 7 Estimation of methane flux into the simulation domain as a boundary condition

Quantity	Unit	Value	Comment
Production per borehole	mio m^3	100	From ExxonMobil catalogue of questions
Production per borehole in methane mass	mio kg	72	Calculated using a density of 0.72 kg/m^3 (atmospheric conditions)
Number of fracturing procedures per horizontal well	–	5	From ExxonMobil catalogue of questions, 5 fractures considered
Production per frack	mio kg	14.4	Production per borehole/fractures per borehole
Fraction of methane not extracted in Haynesville after 10 years	%	20	EIA review
Mass of methane not extracted per frack	mio kg	2.88	20 % of 14.4 mio kg
Production rate per fracture after 10 years for Haynesville	kg/d	1,016.3	EIA review
Time over which methane leaks based on Haynesville values	Years	7.8	Mass of methane not extracted per fracture/ production rate per fracture

Table 8 List of simulations

The parameters of the fault zone and the residual gas (S_{gr}) and liquid (S_{lr}) saturations are varied. The fault zone permeabilities were assumed to be 1×10^{-16} m^2. Each case was further modified at the position of the salt layers, where the permeability was reduced to 5×10^{-18} m^2. For the setting Lünne (depth 1,200 m), the area is located between 850 and 1,050 m depth while for Vechta (depth 3,800 m) it is located between 2,600 and 3,000 m depth

Simulation	Setting	Residual saturations (−)	Fault zone extent	Fault zone permeability (m^2)	Fault zone porosity (−)
1	Lünne	$S_{gr} = 0.01$ $S_{lr} = 0.15$	Homogeneous	1×10^{-16}	0.01
2	Lünne	$S_{gr} = 0.30$ $S_{lr} = 0.15$	Homogeneous	1×10^{-16}	0.01
3	Lünne	$S_{gr} = 0.01$ $S_{lr} = 0.15$	Partially reduced	$1 \times 10^{-16}/5 \times 10^{-18}$	0.01
4	Lünne	$S_{gr} = 0.30$ $S_{lr} = 0.15$	Partially reduced	$1 \times 10^{-16}/5 \times 10^{-18}$	0.01
5	Lünne	$S_{gr} = 0.01$ $S_{lr} = 0.60$	Homogeneous	1×10^{-16}	0.01
6	Lünne	$S_{gr} = 0.30$ $S_{lr} = 0.60$	Homogeneous	1×10^{-16}	0.01
7	Vechta	$S_{gr} = 0.01$ $S_{lr} = 0.15$	Homogeneous	1×10^{-16}	0.01
8	Vechta	$S_{gr} = 0.30$ $S_{lr} = 0.15$	Homogeneous	1×10^{-16}	0.01
9	Vechta	$S_{gr} = 0.01$ $S_{lr} = 0.15$	Partially reduced	$1 \times 10^{-16}/5 \times 10^{-18}$	0.01
10	Vechta	$S_{gr} = 0.30$ $S_{lr} = 0.15$	Partially reduced	$1 \times 10^{-16}/5 \times 10^{-18}$	0.01

Summary and conclusion

In this article, three scenarios are chosen which cover the migration of fracturing fluids, brine and methane on a local and regional scale as well as on a short- and long-term temporal scale. Scenario 1 deals with the short-term movement of fracturing fluid or brine into the overburden induced by high pressures from hydraulic fracturing activities. Scenario 2 shows the long-term horizontal and vertical movement of fracturing fluid and brine in the Münsterland Basin along the Cenomanian–Turonian aquifer and along vertical fault zones connecting the Cenomanian–Turonian aquifer with the shallow Quarternian aquifer system. Long-term methane migration processes are covered in Scenario 3, where methane migrates through a fault zone into the overburden.

In Lange et. al (2013), different settings for locations in North Rhine-Westphalia and Lower Saxony are presented which include a simplified geometry (layer thickness), the parametrisation of the overburden (porosity, horizontal and vertical permeability) as well as the fault zone parametrisation. These settings form the geological model on which

Fig. 18 Comparison of Simulations 1, 2 and 3. **a** The vertical permeability (m^2) for the location Lünne as well as the dimensions of the model domain. **b** The saturation of methane after 100 years for Simulation 3. **c, d** The saturation of methane for Simulations 1 and 2 after 100 years. For these two cases, the fault zone fully penetrates the overburden. Simulations 1 and 2 have differing residual saturations (Simulation 1: 1 %, Simulation 2: 30 %)
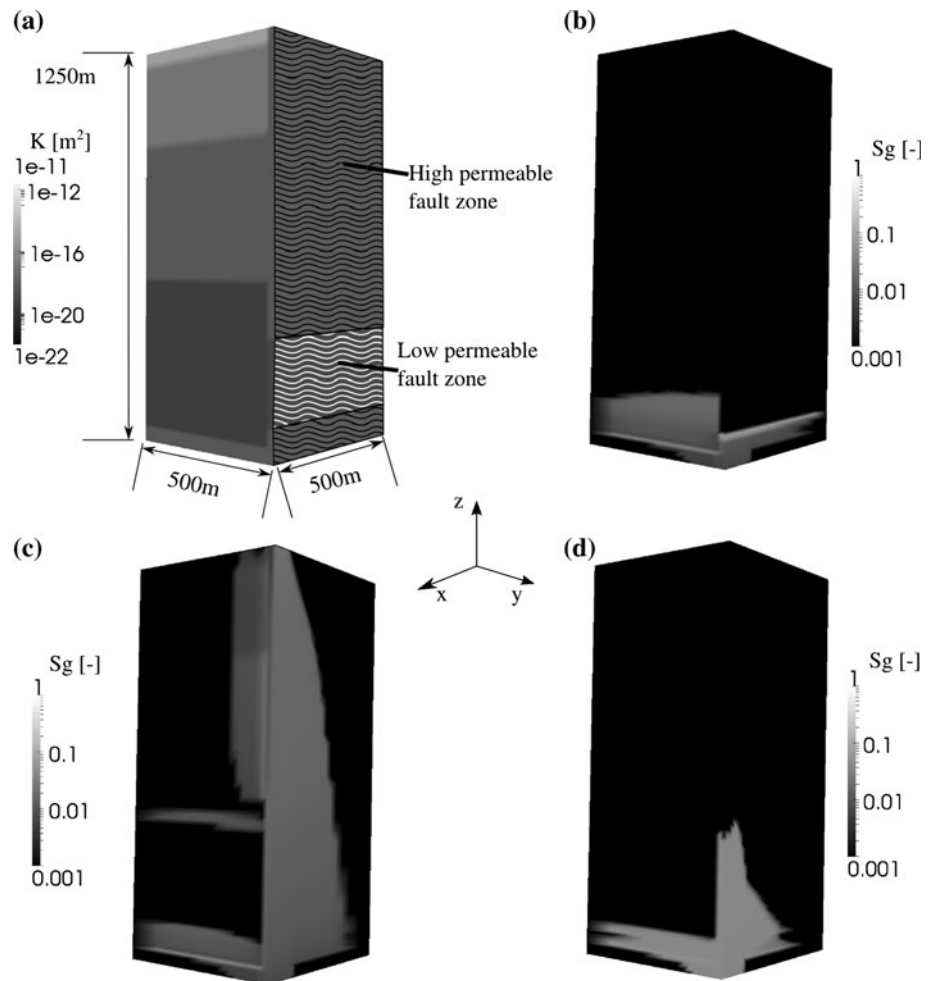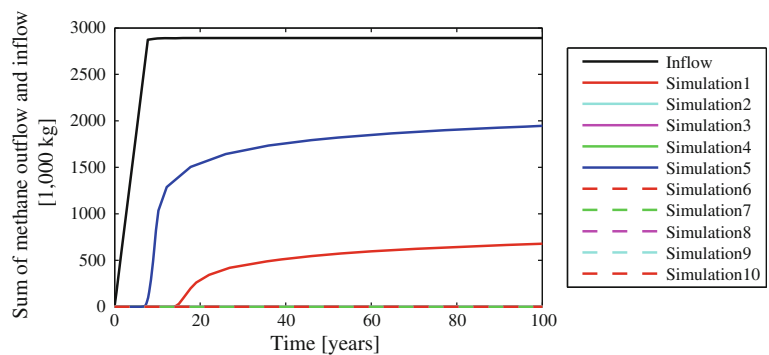
Fig. 19 The amount of methane escaping through the model domain into the shallow Quaternary groundwater system (topmost layer, approximately 50 m below surface) for the different simulations of Scenario 3. "Inflow" refers to the amount of methane entering the model domain from the gas-bearing layer

the numerical model for Scenarios 1 and 3 presented in this work are based on. For Scenario 2, a cross section of the Münsterland Basin parametrised by Lange et al. (2013) is chosen. The results of Scenario 1 show that the short-term propagation of fracturing fluid or brine due to high pressures induced by hydraulic fracturing activities leads to a maximal vertical migration length of 50 m (Setting Bad Laer) above the gas reservoir, if highly permeable fault zones are present. In the considered settings, this is still far from any shallow groundwater aquifers. This result is

based on several conservative assumptions which are shown in Fig. 4. A combination of all these conservative assumptions is considered an unlikely event. No considerable vertical migration is found in the settings in Lower Saxony, since fault zone permeabilities are much smaller than in the Münsterland Basin.

Scenario 2 shows that for the Münsterland Basin the assumption of strong differences in hydraulic head between the Cenomanian–Turonian aquifer and Quarternian aquifer in connection with a fully penetrating and permeable

$(1 \times 10^{-16}$ m^2) fault zone may lead to vertical transport of brine or fracturing fluids, if a preceding contamination of the Cenomanian–Turonian aquifer has occurred. However, the concentrations of the conservative tracer reaching the top layer (Quarternary) are strongly reduced when compared with the initial concentration (factor 4000). Horizontal transport along the Cenoman Turon aquifer can be in the range of tens of meters per year.

In Scenario 3, the amount of methane which migrates into shallow groundwater layers has been calculated for all the settings of Lower-Saxony. In two of the variations, methane actually reaches the shallow layers. This is due to the combination of a fully penetrating fault zone with a low residual gas saturation of the overburden (1 %). However, these results are to be treated with caution. The simulations carried out in this work are not sufficient for a quantitative risk analysis due to the high parameter and scenario uncertainty.

Gaps still remain in the knowledge of the hydraulic fracturing process. The most important gaps and shortcomings are listed below:

– Future work needs reliable field data to calibrate and validate models. To this end, test sites need to be established where monitoring of deep and shallow groundwater through wells may help in recognising the impacts of hydraulic fracturing.
– In regions like the Münsterland Basin, the role of fault zones may have a considerable influence on the migration of fracturing fluid or brine. Possible connections between shallow and deep groundwater should be analysed and quantified through isotope or chemical analysis.
– For a more accurate estimation of the migration of fracturing fluid and brine, models should be set up that include the fractured gas reservoir.
– During the hydraulic fracturing process, brine from the reservoir is displaced by the fracturing fluid. A quantification as to where this water is displaced to under different conditions should also be a focus for future studies.
– Little is known about the release mechanisms of methane from the rock phase. For a quantification of diffuse, long-term methane emissions, these processes need to be understood.
– To get a better understanding of the migration of methane through the overburden representative capillary pressure–saturation relationships, relative permeability–saturation relationships as well as residual gas and water saturations for the different layers of the overburden are needed. The variability of these parameters is great as is their influence on the modelling results. The lack of representative data is

not only relevant for risk estimation related to unconventional gas production, but also for other applications like the storage of methane in sedimentary layers.
– There is a strong need for the improvement of modelling tools which predict the propagation of fractures as well as the flow in fractures, to be able to replace the conservative boundary conditions assumed in this work with more realistic conditions. Only a few geo-mechanical models for fracture propagation exist, but the required input parameters are very hard to obtain, and a validation with field data requires an intensive, very costly and time-consuming monitoring programme.

As mentioned above, this work is not a quantitative risk assessment, but a qualitative evaluation of certain scenarios which we consider to be conservative. Thereby, combinations of unfavourable assumptions and parametrisations which may lead to hazards are identified as a first step, towards a quantitative risk assessment. However, a quantitative risk assessment which should be the main aim of future work in this field has much higher demands, especially on site-specific data, as the estimation of statistical parameter uncertainty requires site-specific parameter distributions (Walter et al. 2012). There is already ongoing research on risk assessment in related fields like CO_2 sequestration. We therefore propose these methodologies to be transferred to risk estimation relating to the use of the hydraulic fracturing method, be it for unconventional gas or enhanced geothermal systems. The overall aim should be to set common and transparent standards for different uses of the subsurface and their involved risks and communicate those to policy makers and stake holders.

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