Universität Stuttgart

Technischer Bericht

TB 09/2014 LH^2 22

Modeling the Migration of Fracturing Fluids into Shallow Groundwater Systems - Literature Review and Numerical Simulations

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Modeling the Migration of Fracturing Fluids into Shallow Groundwater Systems - Literature Review and Numerical Simulations

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1 Introduction

The increased use of high-volume hydraulic fracturing (HF) in connection with horizontal drilling techniques to exploit natural gas from unconventional gas resources like black shales has raised questions in the public whether HF can lead to a contamination of shallow groundwater aquifers or drinking water sources. The possible contamination with HF fluid and brine through pathways of technically induced or natural occurring fractures or faults has herein been one of the concerns. Recently released studies consider a possible contamination (Rozell and Reaven, 2012) or claim to have found evidence (Warner et al., 2012).

This work discusses the article "Potential Contaminant Pathways from Hydraulically Fractured Shale to Aquifers" by Tom Myers (Myers, 2012b) which was published in the November-December 2012 issue of the journal Groundwater (former Ground Water). Myers concludes that hydraulic fracturing fluids could propagate through natural occurring fractures in a few decades to near-surface aquifers. The same issue also includes a critical discussion (Saiers and Barth, 2012) of this article and an Author's Reply (Myers, 2012a). Despite the controversially discussed work of Myers (Myers, 2012b), the authors, who directly addressed him, have the unanimous opinion that a correctly elaborated numerical model has the potential to realistically describe the flow regime before, during and after a HF process, and that such a model could be crucial for an improved risk assessment of HF treatment. The purpose of this work is to point out ways to create a relatively straight forward numerical model, which is able to illustrate the conceptual flow behavior of brine and HF fluid over long periods of time. The model should be a first tool to assess parameters and phenomena which are crucial for the flow process when modeling a HF treatment. In Section 2 we discuss the assumptions made in (Myers, 2012b). In Section 3 we describe the relevant physical processes and and explain which processes we include into our model setup. In Section 4 we take a closer look at the assumption of persistent vertical head gradients leading to constant fluxes from deep layers into more shallow layers with help of a simple algebraic estimation. Finally, we setup a model for simulating the HF process in Section 5. Here we investigate the influence of the injection itself as well as the buoyancy effects caused by the injection of water based fracturing fluid into highly saline formation fluid on a possible vertical migration of fracturing fluids.

2 Discussion of Myers' Model

Saiers and Barths' critiques are enforced by a technical rebuttal (Carter et al., 2013) and a more general paper (Flewelling and Sharma, 2013) about upward migration of fracturing fluids and brine. These articles point out several shortcomings and oversimplifications of Myers' model, especially in lithostratigraphy, hydrogeology and model parametrization. A further discussion of Myers article (Cohen et al., 2013) exposes additional mathematical and typographical errors.

Here, we state and order the critiques mentioned in the stated articles:

- neglect of density driven flow,
- restricted model domain,
- unrealistic expansion, orientation and hydraulic connectivity of a fault zone,
- oversimplified modeling of the HF process,
- non-consideration of multi-phase correlated phenomena such as water-undersaturated formations, high capillary forces and void-space imbibition in shales,
- absence of rock heterogeneities,
- absence of pressure gradients during the extraction phase,

- unlikelihood of the long-time existence of vertical head gradients in high permeable shale formations.

3 Relevant Phyiscal Processes and Implementation

In the following, each point of critique is reviewed and the incorporation into our model is discussed.

Salinity and Temperature

Myers does not implement any kind of salinity or temperature gradients, although he acknowledges their occurrence.
High salinity values, up to 400,000 ppm, (Bassett and Bentley, 1983; Hanor, 1983) can be found in deep shale aquifers which have a significant effect on the water density. The existence of high salinity and thus density gradients can provoke serious consequences to the overall flow regime (Birkholzer et al., 2011; Oldenburg and Rinaldi, 2010) and creates effects such as convection (Simmons et al., 2008). Naturally occurring temperature gradients (Ajayi et al., 2011; Shope et al., 2012) cause changes in water properties, especially influencing the water density at higher temperatures.
One of the essential changes in regard to Myers' model is the implementation of a salinity gradient into our model. Additionally a constant temperature gradient is integrated, but without considering energy fluxes. Therefore the temperature influences fluid properties with changing depth.

Effects of Variable Density on Flow

Due to the previously discussed neglect of density gradients, Myers' model is not able to account for density driven flow.
A first estimate whether the criteria for the onset of density driven flow are met can be evaluated with the dimensionless Rayleigh number Ra (Horton and Rogers, 1945; Lapwood, 1948). Basically, the number describes the ratio of gravitational or buoyant flow, including a term for the fluid density difference, and diffusive or dispersive flow. Convection, driven by salinity gradients, was already observed and described for example in high permeable shales (Sharp et al., 2001) or in vertical fractures intersecting a low permeable shale layer (Simmons et al., 2008). High density differences may also arise when injecting water based HF fluid into high saline shale formations, thereby creating conditions for convective flow.
The decision to include salinity and temperature gradients into our model gives us the opportunity to describe more realistic flow conditions.

Boundary Conditions and Model Domain

Myers' model domain consists out of a cuboid with a base area side length of 450 m and a height of 30 m shale and 1500 m overburden. Dirichlet boundary conditions specify a higher potential (constant head) at the bottom than at the top. The lateral sides are defined as no-flow boundary conditions.
This kind of geometry and boundary constellation inevitably leads to upward directed flow (Saiers and Barth, 2012; Cohen et al., 2013; Carter et al., 2013) and neglects the general flow tendency parallel to the direction of bedding in high permeable layers (Freeze and Witherspoon, 1967). Especially during the injection of hydraulic fracturing fluid, the no-flow boundaries cause unrealistic pressure gradients (Saiers and Barth, 2012).
To reduce the influence of the boundary conditions during the injection, we increased the area of the model domain extensively. However all lateral boundaries are still assigned as no-flow conditions,

because open boundaries have the potential to induce artificial pressure gradients. More realistic boundary conditions can only be applied when modeling a specific regional area with available topographic and hydrogeologic data.

Fault Zone

A strictly vertical fault zone, extending from right above the shale up to the surface with a permeability 10 to 1000 times higher than the surrounding rock is used in Myers model.
A high permeable connection between the gas bearing formation and shallow aquifers or the surface is regarded to be unrealistic, owing to the fact that the drinking water overlying the Marcellus Shale is potable (Saiers and Barth, 2012; Carter et al., 2013). Nevertheless, several papers and microseismic studies report fault zone reactivation in the proximity of conducted HF operations, indicating HF near fault zones takes place (Soltanzadeh and C. Hawkes, 2009; Cipolla et al., 2011). These fault zones have the potential to function as conduits for gas or brine over long periods of time (Person et al., 2008; Simmons et al., 2008).
To define the geometry and the parameters of a realistic worst-case fault zone in an easy numerical model, one has to rely mostly on pure assumptions. For the sake of simplicity a strict vertical, homogeneous fault zone from right above the shale to a depth of 200 m (Williams, 2010) where the base of freshwater aquifers can appear was assumed.

Hydraulic Fracturing Process

The HF process in Myers' model was approximated with a constant injection of 15 million liters over a period of five days.
This approach disregards the more complex management of alternating injection rates and the HF of isolated segments (Arthur et al., 2008; Saiers and Barth, 2012).
In our model we accepted conservative assumptions and simplifications to implement the HF process. We assumed the area of injection to be a isolated segment of an HF operation and therefore reduced the time and injected fracturing fluid volume drastically.

Multi-phase Phenomena

Myers only considers the flow of water in a fully saturated porous media.
The occurrence of natural gas or nonaqueous-phase liquids in deep shale formations (Milici and Swezey, 2006; Ejofodomi et al., 2011) creates complex multi-phase systems. For example, low water saturation in shales (Bruner and Smosna, 2011; McKeon, 2011), sometimes to such an extend that no free water is present (Stephens, 1996), leads to a very low water permeability. Furthermore, low water saturation induces high capillary pressure, trapping imbibed water in the shale matrix (Byrnes, 2011; Engelder, 2012). These phenomena pose an additional obstacle for vertical flow of brine or HF fluid.
Although the issue should be correctly addressed with a multi-phase approach, we decided to use a single phase model, because we

- are interested in worst case scenarios,
- have no reliable data for all multi-phase flow correlated parameters and
- attempt to create a straight forward model to evaluate basic and crucial parameters.

Heterogeneity

Myers' model domain is represented by two homogeneous layers which only vary in permeability.
The Marcellus Shale itself, and especially the overlying rock, consisting largely out of horizontal layers of shale, mudstone, siltstone, limestone and sandstone (Milici and Swezey, 2006; Harper and Kostelnik, 2008) creates a highly heterogeneous geological system.
The heterogeneity and thus the variation of the permeability and porosity over an extensive geological domain is beyond questioning. However, our interests are mainly focused on building a model in which the impacts of a single parameter is easily determined and thus complex, heterogeneous geological structures are not considered here.

Pressure Gradients During Extraction Phase

Myers does not recognize occurring pressure gradients during the production phase of a gas well directing fluids towards the gas bearing shale.
Production curves of the Marcellus Shale have a best fit with a power-law rate decline curve (Engelder, 2009). Therefore, especially during the first years of production, a low pressure zone in the targeted formation could force natural gas, brine and HF fluid towards the well.
Our model is designed to calculate long term fluid migration due to the fact that velocities in low-permeable porous media are very small. Furthermore, rather then computing realistic contaminant concentrations, our model has the purpose of estimating the dominant long term flow behavior of worst case scenarios.

Coexistence of High Permeabilities and Vertical Head Gradients

Myers accepts the long time persistence of a vertical head gradient in co-occurrence with low rock permeabilities in and above the shale.
Northern parts of the Marcellus formation are overpressured (Sumi, 2008; Hill et al., 2004). In order to endure such a condition, the overlying rock permeability has to be very low, and potentially existing vertical fluxes are small (Flewelling and Sharma, 2013). Frequently alleged reasons for this effective hydraulic isolation are the existence of unconventional gas resources and overlying non-contaminated drinking-water aquifers in areas of over-pressured gas bearing formations (Flewelling and Sharma, 2013; Carter et al., 2013).
The vertical head gradients are discussed in more detail in Section 4 using a simple algebraic estimation.

4 One Dimensional Model

Myers model is constructed in such a way that a continuous vertical flow is present under all conditions. This vertical flux is the result of 30 m piezometric head, representing the overpressure in the shale, added to the hydrostatic pressure at the bottom of the domain.
The question which should be asked now is: Under what circumstances can such a continuous flux be obtained when salinity and temperature gradients are present?
To understand the basic impact of a density and temperature gradient on vertical flow, it is sufficient to examine a simple 1D model:
The top and bottom boundaries are constructed as Dirichlet conditions at which the pressure and the salinity are constant. An atmospheric pressure of 0.1 MPa, a salinity of 0.2 grams of salt per liter (drinking water), a hydrostatic pressure plus 30 m of piezometric head (overpressure) and an increased salinity are defined at the top and bottom boundary respectively. Initially, the whole domain is saturated with pure water (no salt). A geothermal gradient of 30 °C km^{-1} without considering energy fluxes is applied.
Under such conditions low saline fluid leaves the model domain at the top and high saline brine enters the domain from the bottom. Therefore, the overall salinity and thus density inside the model domain increases until the hydraulic potential and therefore the advective flux becomes zero. At this point of time, the fluid inside the tube stops moving and a new hydrostatic equilibrium is reached (Oldenburg and Rinaldi, 2010). A change in permeability only changes the magnitude of the vertical flux and the time until a new equilibrium is obtained.
Figure 1 shows a sketch of the model in 2D with the dotted line marking the propagation height of the high density brine front after meeting the new equilibrium (t$_{end}$).

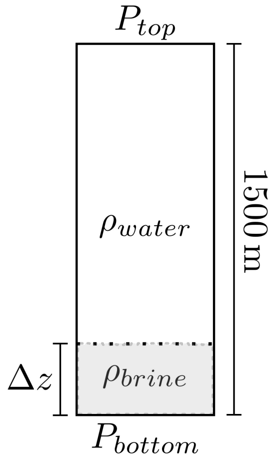

Figure 1: Model domain of the basic model in 2D

The propagation height Δz [m] can be estimated with the help of a simple algebraic formula by stating the pressure at the bottom P$_{bottom}$ at the beginning (t$_{begin}$):

$$P_{bottom} = (H + Pot) \cdot \rho_{water} \cdot g + P_{top}, \qquad [Pa] \qquad (1)$$

and at t$_{end}$:

$$P_{bottom} = (H - \Delta z) \cdot \rho_{water} \cdot g + \Delta z \cdot \rho_{brine} \cdot g + P_{top}, \qquad [Pa] \qquad (2)$$

where H [m] denotes the domain height, Pot [m] the added piezometric head at the bottom, ρ_{water}

[$kg\,m^{-3}$] the water density, g [$m\,s^{-2}$] the gravity, P_{top} [Pa] the pressure at the top and ρ_{water} [$kg\,m^{-3}$] the brine density. By equating the right hand side of these two equation, the following expression is obtained:

$$\Delta z = \frac{\rho_{water} \cdot Pot}{\rho_{brine} - \rho_{water}}. \qquad [m] \qquad (3)$$

The propagation height Δz can then be calculated in a non-recursive manner using the relationship of Batzle and Wang (1992) for the brine density.

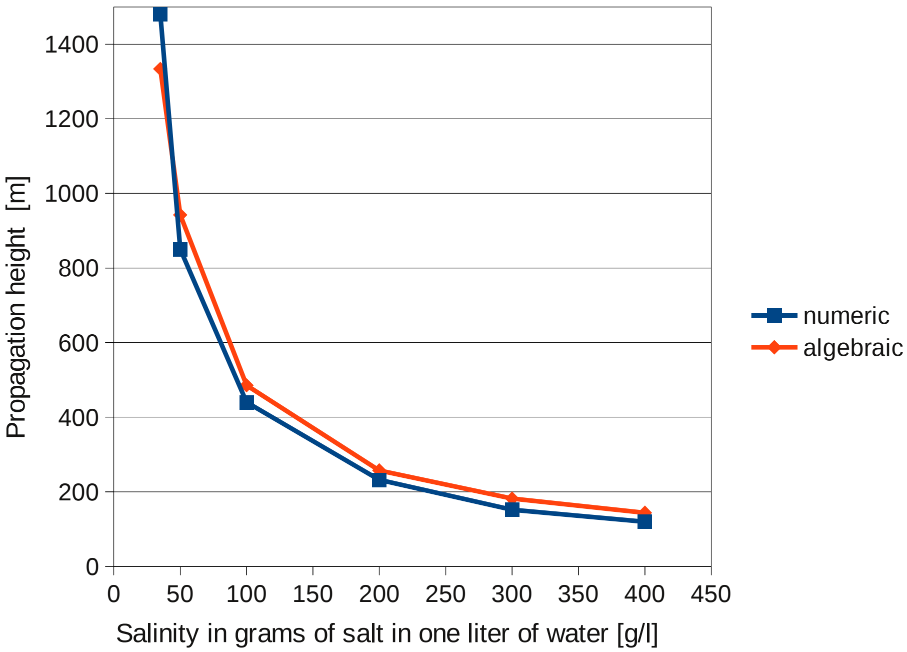

Figure 2: Brine propagation height at the new hydrostatic equilibrium for different salinities calculated numerically and algebraically.

Figure 2 shows the propagation height of the brine front for different salinities after reaching the new hydrostatic equilibrium calculated with the above stated formula as well as with a numerical 1D model. The numerical results are obtained with the numerical simulator $DuMu^x$ (Flemisch et al. (2010), `http://www.dumux.org`). For the simulations, we use an isothermal one-phase two component model, considering water and salt as components. For spatial discretization, the BOX method is used, which is a node-centered finite volume method based on a finite element grid (Helmig, 1997). For temporal discretization, a fully implicit scheme is applied using the Newton method to handle the system of non-linear partial differential equations. For calculating the brine density and dynamic viscosity we use the relationship by Batzle and Wang (1992).

The algebraic and the numerical results match quite well, especially in cases of high salinity. The overestimation of propagation height in the algebraic case originates from a uniform brine density assumption which neglects the impact of temperature and pressure on the fluid density.

A continuous vertical flow over a distance of about 1500 m can be observed when the applied overpressure is able to push the high density brine front all the way to the top. With an overpressure of 30 m, this condition can be obtained with a brine salinity of approximately 35 $g\,l^{-1}$.

These simple considerations show that a continuous vertical flux calls either for a very small density gradient which is unlikely when observing deep shale formations, or for an highly over-pressured shale.

Similar considerations in conjunction with the carbon capture and storage (CCS) technology can be found in Birkholzer et al. (2011) and Oldenburg and Rinaldi (2010).

5 Three Dimensional Model

The purpose of the three dimensional model is to simulate the HF process with different injection rates in order to look at the effects of the injection on the vertical migration of the fracturing fluid.

Model Setup

An isothermal, one phase, three component model setup in $DuMu^X$ with similar spatial and temporal discretization as described in Section 4 is used for all further considerations. The liquid phase consists of the three components water, dissolved salt and a conservative tracer representing chemicals present in the injected fracturing fluid.
The geological setting used here is closely related to the setup presented in (Myers, 2012b). Due to symmetry reasons only a quarter of the whole domain is used for the simulations (see Fig 3). This model domain is defined as a 1.6 km high, 11.2 km long and wide cuboid which is divided into three geological layers (see Fig. 3). The lowermost 100 m thick ground layer represents a section of the rock formations underlying the Marcellus Shale, the middle 30 m thick layer the actual Marcellus Shale and the uppermost 1470 m thick layer all overlying rocks. All layers are homogeneous, isotropic and have a horizontal alignment. A three meter wide and 225 m deep fault zone with an increased permeability expands vertically from right above the shale to a depth of 200 m. The spatial mesh discretization focuses on the region of the frontal left bottom corner where the fracturing fluid is going to be injected with logarithmically increasing elements in all three directions.
At the top and bottom boundaries a Dirichlet condition is applied at which the pressure and the salinity is specified. The lateral Neumann no-flow boundary conditions create an enormous tube where the frontal and right boundaries function as symmetry axis. It was decided against open lateral boundary conditions, which allow distinctive horizontal flow, because the transient salinity distribution inside the domain generates artificial boundary effects.
A constant temperature gradient of $30\,^{\circ}\mathrm{C\,km^{-1}}$ is assumed. The parameters of interest which are constant for all further considerations are listed in Table 1. The very high permeability value for the shale layer is adopted from Myers considerations (Myers, 2012b), although the majority of shale permeabilities are assumed to be several orders of magnitude smaller (Neuzil, 1994).

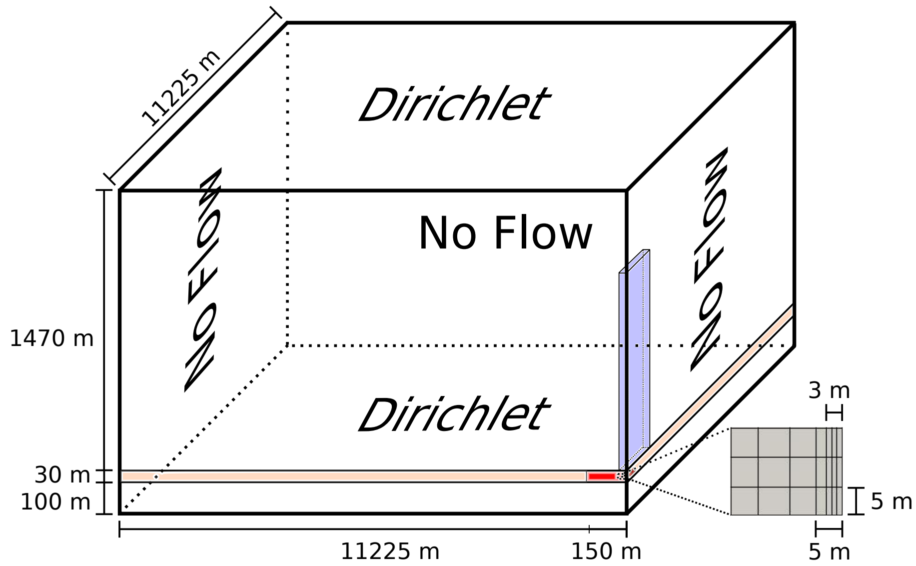

Figure 3: Model domain of the three dimensional model (not to scale). The brown layer illustrates the Marcellus Shale with the red part showing the area in which the permeability is increased by HF; the blue block represents the fracture. The grid cutout shows the mesh on the right hand side inside the Marcellus Shale at its finest resolution. Note that the frontal boundary condition is not labeled but is also defined as a no-flow condition.

Table 1: Constant parameters

Parameter		**Value**
Porosity layers	ϕ	0.1
Permeability ground layer	k_g	$1.18^{-15}\,\mathrm{m}^2$
Permeability shale layer	k_{sh}	$1.18^{-15}\,\mathrm{m}^2$
Permeability shale layer in HF area (during, after HF)	k_{sh}	$1.18^{-13}\,\mathrm{m}^2$
Permeability overburden layer	k_{ov}	$1.18^{-13}\,\mathrm{m}^2$
Permeability fault zone	k_{fault}	$1.18^{-11}\,\mathrm{m}^2$
Pressure on the top	p_{top}	100,000 Pa
Temperature on the top	T_{top}	10 °C
Temperature on the bottom	T_{bottom}	58 °C
Salinity on the top and initial	Sal	$0.2\,\mathrm{g\,l}^{-1}$
Salinity bottom	Sal	$100\,\mathrm{g\,l}^{-1}$
Brine Propagation height (see Figure 2)	-	450 m
Density fracturing fluid	ϱ_{ff}	1000 kgm^{-3}
Mollecular diffusion coefficient salt	D^{Salt}	$1.0^{-9}\,\mathrm{m}^2\,\mathrm{s}^{-1}$
Mollecular diffusion coefficient tracer	D^{Tracer}	$1.0^{-9}\,\mathrm{m}^2\,\mathrm{s}^{-1}$

Modeling of the Hydraulic Fracturing Process

The HF of the shale only takes place over a horizontal length of 150 m. Therefore, contrary to Myers, we consider the HF treatment as a sealed single stage treatment and the time and volume (note also the quartering of the domain) of the injected fluid are reduced drastically. Two injection scenarios are considered in this work (A and B). In Case A 500,000 liters of fracturing fluid (Arthur et al., 2008) are injected with a constant rate into the middle of the shale over a five hour stress period. In Case B according to (Myers, 2012b) 3,750,000 l are injected during a five day injection period. The fracturing fluid is designed as a mixture consisting of 99 % water and 1 % conservative tracer, representing different, possibly occurring chemicals (NYSDEC, 2011). At the beginning of the HF process, the intrinsic permeability of the shale layer is increased in the vicinity of the injection (over whole shale thickness and 15 m deep) by a hundredfold. It is assumed that no out of formation fracturing occurs, although this phenomenon was observed multiple times (Fisher and Warpinski, 2011). Furthermore, a higher increase of the shale permeabilities due to HF can be found (Zielinski and Nance, 1979) but shall be neglected in our considerations. After the injection has ended, a 60 day period starts, in which 20 % of the previous injected fluid is extracted with a constant rate to simulate the flowback (Myers, 2012b, and references herein).

Model Initialization

To establish an initial state for the pressure and the salinity, model results in the state of the new hydrostatic equilibrium from the basic 1D model are taken and implemented into the 3D model. Ten years of initialization time are then followed by the HF process and a post injection period of 200 years in which the propagation of the tracer plume can be examined.

Variable Parameters

Only the injection duration and the injection volume of the HF are varied to analyze their impact on the flow regime. The two cases are shown in Table 2.

Table 2: Paramater values of the sensitivity analysis

Case number	Injection duration [h]	Injection volume [l]
A	5	500,000
B	120	3,750,000

Results

Due to the fact that we start our HF process in a state of hydrostatic equilibrium and the applied overpressure is consumed by keeping the heavy brine front elevated, the only forces which lead to an upward migration of fracturing fluid into shallower aquifers are advective forces arising from the injection and buoyancy forces, caused by density differences between the formation and fracturing fluid. The injected fracturing fluid consists mostly of water, so an analogous density is assumed.

In Figure 4, the section of the model domain in which the hydraulic fracturing fluid has been injected is shown for different points in time for the Cases A and B. In Case A, the tracer does not migrate out of the shale and into the high permeable fault zone. In Case B where a larger volume of fracturing fluid is injected, the tracer is able to migrate out of shale and into the overburden. The density differences between injected and surrounding fluid and therefore the buoyancy forces become smaller until they

diminish and a new hydrostatic equilibrium is reached (see Figure 4 after 200 years) after a vertically covered distance of only 5 m for Case A and 50 m for Case B.
Generally, the influence of the advective forces due to the injection on the vertical migration is rather small due to its short period of impact. This can be seen in Figure 4 for Cases A and B after 10 years, where no significant vertical migration has occurred.
The vertical migration distance due to buoyancy forces is controlled by two factors: (i) density of the surrounding fluid where the density is varying over depth due to the salinity distribution and the geothermal gradient and (ii) mixing between fracturing and formation fluid. Factor (i) is negligible here since the salinity is constant at a value of 100 g/l up to 450 m above the shale (see Table 1). Since an isothermal model is used the geothermal temperature gradient is constant as well. Mixing (ii) is the main factor influencing the vertical migration distance. With an increased volume of low density fracturing fluid injected the vertical migration height increases as the mixing distance (i.e. the vertical distance until mixing between the formation fluid and the fracturing fluid neutralizes the buoyancy forces) also increases. This can be explained by with the help of the Rayleigh number which relates the buoyancy or gravitational flow to the dispersive flow:

$$Ra = \frac{\Delta \varrho k g d}{\mu D} \tag{4}$$

Here $\Delta \varrho$ is the density difference between the two fluids (in this case only caused by different salinities), k is the permeability, d is a characteristic length (height) and D is the diffusion which in this case comprises the effective molecular diffusion as well as the numerical dispersion caused by the spatial and temporal discretization of the problem. In the extreme case of fracturing and formation fluid being two separate and immiscible phases there would be no mixing and the fracturing fluid would gradually rise to the top of the domain. Therefore, the limited vertical migration distance observed here will most likely also be very sensitive to numerical dispersion and therefore the grid resolution. However, a grid convergence study was not conducted here.
Considering our simulation results, the fault zone only plays a minor role in the final propagation height. This high permeable zone is only able to increase the flow velocity as long as buoyant fluxes are present.

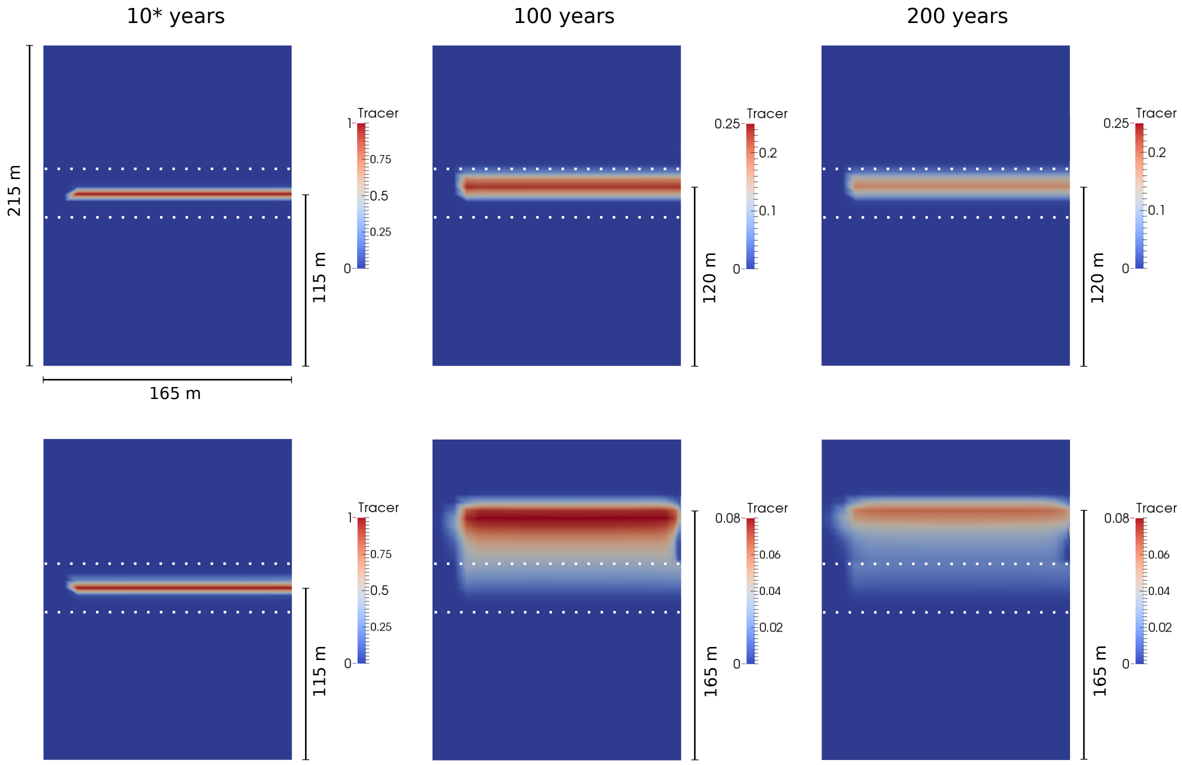

Figure 4: Tracer propagation heights for case A (top) and B (bottom) for different times (* after injection and flowback phase). White dotted line illustrates the shale layer. Note: different tracer scales were used in the result images.

6 Summary and Outlook

Hydraulic fracturing bears potential risks of contaminating groundwater aquifers due to flow of non-recovered fracturing fluid or displaced brine through normal porous media or natural occurring fault zones (Rozell and Reaven, 2012; Warner et al., 2012). The article "Potential Contaminant Pathways from Hydraulically Fractured Shale to Aquifers" (Myers, 2012b) claims strong evidence for vertical contaminant flow and concludes, based on model results, that shallow aquifers could be polluted by hydraulic fracturing fluid traveling through natural occurring fractures in tens of years. Several articles (Saiers and Barth, 2012; Carter et al., 2013; Flewelling and Sharma, 2013; Cohen et al., 2013) already discussed and criticized Myers work, but failed to implement their critiques into an independent numerical model.
Therefore a simple, straightforward numerical model based on Myers' considerations, while also incorporating some of the expressed concerns is built. The most notable changes are:

- the implementation of salinity and temperature gradients,
- the consideration of convective effects and
- an extension of the restricted model domain.

However, this model does not make any claim for completeness. We are aware of simplifications and non-considerations, especially with regard to

- multi-phase flow phenomena,

- local and global heterogeneities,
- pressure gradients during the extraction phase,
- long-time coexistence of vertical head gradients in high permeable shale formations and
- neglect of non-isothermal effects on buoyant flow.

As a first important step to understanding the overall flow behavior in deep saline basins, the impact of the salinity and temperature gradient implementation in a tube-like model domain with an overpressure at the bottom boundary is described. Therefore, a very simple algebraic and a numerical 1D model show the establishment of a new hydrostatic equilibrium for different salinity cases, which leads to the conclusion that continuous vertical flow, as described by Myers, seems unlikely.
On this basis, a more sophisticated model is built (see Section 5), to describe the flow regime mainly during and after a HF process.
The model calculates fracturing fluid propagation heights for two different injection scenarios. The highest propagation height caused by buoyant forces adds up to 50 m after 100 years (Case B).
However, this result is most likely very sensitive to the grid resolution as numerical dispersion causes mixing which reduces buoyant forces. Therefore, care should be taken for this kind of problems where flow is strongly controlled by the Rayleigh number so that the results are independent of the grid resolution.

In summary, the conducted work confirmed and discussed the following points:

- Salinity gradients have the potential to extensively influence the overall flow regime.
- Density differences between the fracturing and the formation fluid should not be neglected for migration scenarios.
- Generally, the influence of the advective forces due to the injection on the vertical migration is rather small due to its short period of impact.

A promising numerical model is currently developed by the Lawrence Berkeley Laboratory under the coordination of the Environmental Protection Agency (EPA) of the United States of America (EPA, 2012). This model incorporates all stated critiques and has the aim to rebuild subsurface conditions, the HF process and fracture propagation in great detail and has the potential to produce realistic and reliable results.

References

Ajayi, B., Walker, K., Wutherich, K., and Sink, J. (2011). Channel hydraulic fracturing and its applicability to the Marcellus Shale. Paper SPE 149426 prepared for the presentation at the SPE Eastern Reginal Meeting.

Arthur, A. J. D., Consulting, A. L. L., Bohm, B., Layne, M., and Ph, D. (2008). Hydraulic Fracturing Considerations for Natural Gas Wells of the Marcellus Shale. *The Groundwater Protection Council, Cincinatti, Ohio.*

Bassett, R. L. and Bentley, M. E. (1983). Deep Brine Aquifers in the Palo Duro Basin : Reginal Flow and Geochemical Constraints. (130).

Batzle, M. and Wang, Z. (1992). Seismic properties of pore fluids. *Geophysics*, 57(11):1396–1408.

Birkholzer, J. T., Nicot, J. P., Oldenburg, C. M., Zhou, Q., Kraemer, S., and Bandilla, K. (2011). Brine flow up a well caused by pressure perturbation from geologic carbon sequestration: Static and dynamic evaluations. *International Journal of Greenhouse Gas Control*, 5(4):850–861.

Bruner, K. and Smosna, R. (2011). A Comparative Study of the Mississippian Barnett Shale , Fort Worth Basin , and Devonian Marcellus Shale , Appalachian Basin.

Byrnes, A. P. (2011). Role of Induced and Natural Imbibition in Frac Fluid Transport and Fate in Gas Shales.

Carter, K. M., Kresic, N., Muller, P., and Vittorio, L. F. (2013). Technical Rebuttal to Article Claiming a Link between Hydraulic Fracturing and Groundwater Contamination. pages 1–13.

Cipolla, C., Maxwell, S., Mack, M., and Downie, R. (2011). A Practical Guide to Interpreting Microseismic Measurements. *North American Unconventional Gas Conference and Exhibition, Society of Petroleum Engineers, The Woodlands, Texas, USA.*

Cohen, H. a., Parratt, T., and Andrews, C. B. (2013). Potential contaminant pathways from hydraulically fractured shale to aquifers. *Ground water*, 51(3):317–9; discussion 319–21.

Ejofodomi, E., Baihly, J., Malpani, R., Altman, R., Schlumberger, Huchton, T., Welch, D., and Zieche, J. (2011). Integrating All Available Data To Improve Production in the Marcellus Shale. Paper SPE 144321 presented at SPE North American Unconverntional Gas Conference and Exhibition, The Woodland, Texas.

Engelder, T. (2009). Marcellus 2008: Report card on the breakout year for gas production in the Appalachian Basin. (August).

Engelder, T. (2012). Capillary tension and imbibition sequester frack fluid in Marcellus gas shale. *Proceedings of the National Academy of Sciences of the United States of America*, 109(52):E3625; author reply E3626.

EPA (2012). Study of the Potential Impacts of Hydraulic Fracturing on Drinking Water Resources Progress Report. (December).

Fisher, K. and Warpinski, N. (2011). SPE 145949 Hydraulic Fracture-Height Growth : Real Data. (November).

Flemisch, B., Darcis, M., Erbertseder, K., Faigle, B., Mosthaf, K., Lauser, A., Müthing, S., Nuske, P., Tatomir, A., Wolf, M., and Helmig, R. (2010). DuMux: DUNE for Multi-Phase, Component, Scale, Physics,... Flow and Transport in Porous Media. *Advances in Water Resources.*

Flewelling, S. a. and Sharma, M. (2013). Constraints on Upward Migration of Hydraulic Fracturing Fluid and Brine. *Ground water*, pages 1–11.

Freeze, R. and Witherspoon, P. (1967). Theorethical analysis of reginal groundwater flow: 2. Effect of water-table configuration and subsurface permeability variation. *Water Resources Research*, 3(2):623–634.

Hanor, J. (1983). Fifty years of development of thought on the origin and evolution of subsurface sedimentary brines. *Revolution in the Earth Sciences: Advances in the Past Half-Century*, pages 99–111.

Harper, J. A. and Kostelnik, J. (2008). The Marcellus Shale Play in Pennsylvania. *Pennsylvania Geological Survey.*

Helmig, R. (1997). *Multiphase flow and transport processes in the subsurface : A contribution to the modeling of hydrosystems.* Springer.

Hill, D. G., Lombardi, T. E., and Martin, J. P. (2004). Fractured Shale Gas Potential in New York. pages 1–49.

Horton, C. W. and Rogers, F. T. (1945). Convection Currents in a Porous Medium. *Journal of Applied Physics*, 16(6):367.

Lapwood, E. R. (1948). Convection of a fluid in a porous medium. *Mathematical Proceedings of the Cambridge Philosophical Society*, 44(04):508.

McKeon, M. (2011). Horizontal fracturing in shale plays, Presentation to the Eastern Section of the Petroleum Technology Transfer Council, New Philadelphia, OH.

Milici, B. R. C. and Swezey, C. S. (2006). Assessment of Appalachian Basin Oil and Gas Resources : Devonian Shale – Middle and Upper Paleozoic Total Petroleum System. Technical report, USGS.

Myers, T. (2012a). Author's Reply. *Ground Water*, 50(6):828–830.

Myers, T. (2012b). Potential Contaminant Pathways from Hydraulically Fractured Shale to Aquifers. *Ground water*, 50(6):872–882.

Neuzil, C. E. (1994). How permeable are clays and shales? 30(2):145–150.

NYSDEC (2011). Revised Draft Supplemental Generic Environmental Impact Statement On The Oil, Gas and Solution Mining Regulatory Program. Technical report, New York State Department of Environmental Conservation.

Oldenburg, C. M. and Rinaldi, A. P. (2010). Buoyancy Effects on Upward Brine Displacement Caused by CO2 Injection. *Transport in Porous Media*, 87(2):525–540.

Person, M., Banerjee, A., Hofstra, A., Sweetkind, D., and Gao, Y. (2008). Hydrologic models of modern and fossil geothermal systems in the Great Basin: Genetic implications for epithermal Au-Ag and Carlin-type gold deposits. *Geosphere*, 4(5):888–917.

Rozell, D. J. and Reaven, S. J. (2012). Water pollution risk associated with natural gas extraction from the Marcellus Shale. *Risk analysis : an official publication of the Society for Risk Analysis*, 32(8):1382–93.

Saiers, J. E. and Barth, E. (2012). Potential contaminant pathways from hydraulically fractured shale aquifers. *Groundwater*, 50(6):826–828.

Sharp, J., Fenstemaker, T., Simmons, C., McKenna, T., and Dickinson, J. (2001). Potential Salinity-Driven Free Convection in a Shale-Rich Sedimentary Basin: Example from the Gulf of Mexico Basin in South Texas. *AAPG*, 85:2089–2110.

Shope, E. N., Reber, T. J., Stutz, G. R., Aguirre, G. A., Jordan, T. E., and Tester, J. W. (2012). Geothermal Resource Assessment: A detailed approach to low-grade resources in the states of New York and Pennsylvania.

Simmons, C. T., Sharp, J. M., and Nield, D. a. (2008). Modes of free convection in fractured low-permeability media. *Water Resources Research*, 44(3):n/a–n/a.

Soltanzadeh, H. and C. Hawkes (2009). Assessing fault reactivation tendency within and sourrounding porous reservoirs during fluid production or injection. *International Journal of Rock Mechanics and Mining Sciences*, 46(1):1–7.

Stephens, D. (1996). *Vadose Zone Hydrology.* CRC Press.

Sumi, B. L. (2008). Shale Gas : Focus on the Marcellus Shale For the Oil & Gas Accountability Project. (May).

Warner, N. R., Jackson, R. B., Darrah, T. H., Osborn, S. G., Down, A., Zhao, K., White, A., and Vengosh, A. (2012). Geochemical evidence for possible natural migration of Marcellus Formation brine to shallow aquifers in Pennsylvania. *Proceedings of the National Academy of Sciences of the United States of America*, 109(30):11961–6.

Williams, J. H. (2010). Evaluation of Well Logs for Determining the Presence of Freshwater, Saltwater, and Gas above the Marcellus Shale in Chemung, Tioga, and Broome Counties, New York.

Zielinski, R. and Nance, S. (1979). Physical and Chemical Characterization of Devonian Gas Shale.