Hydrology and Earth System Sciences

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Discussions

Interactive comment on "Effective damage zone volume of fault zones and initial salinity distribution determine intensity of shallow aquifer salinization in geological underground utilization" *by* M. Langer et al.

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The authors would like to thank the three anonymous referees for the careful reading of our manuscript. We deeply appreciate all the valuable comments and suggestions, which helped us a lot to improve the quality of the paper. We have responded to all comments made and will consider them in our revised manuscript.

On behalf of all co-authors, Elena Tillner

Answers to comments of anonymous Referee #3

RC (Page 5704) Line 7: delete "by" Line 8: what is an "ambient" fault zone ? Line 16: I would try to avoid "these" here as it is somewhat ambiguous. How about "Different boundary conditions proved to have a crucial impact..."? Line 17 "the fluid mass that migrates upward corresponds to the mass of injected fluid"? Lines 16 – 27: this paragraph is too unstructured, too many new scenarios with details (short faults, additional reservoirs,...) are being introduced. Even after reading the entire paper, I found this difficult to follow.

AC (Page 5704) Line 7: "by" will be deleted. Line 8: "ambient" replaced by regional. Line 16: beginning of the sentenced will be revised as suggested by referee. Line 17: sentence will be revised as suggested by referee. Lines 16-27: paragraph will be rewritten for a better understanding, misleading information will be deleted.

RC (Page 5705) Line 3: the initial salinity distribution is discussed, but its effect is not tested in the paper. Therefore, this statement should be softened. Line 11: not sure how "whereby" fits here Line 13: Not sure how the extent and storage capacity of formation leads them to be filled with freshwater. Line 13: above "saline aquifers" here "shallow aquifers". Should be consistent. I think shallow gives the wrong impression. Most would not consider an 800m deep aquifer "shallow". Line 14: "also comprise" Line 14: this sounds as if the storage and freshwater formation are the same. While this is certainly possible (e.g., Ketzin and Kevin Dome), in most cases the injection formation will contain brine. The case modeled here certainly falls in the saline formation category, so I'm not sure why the description is confused here. Line 20: would be good to have some references here. Line 25: The Person et al (2010) paper should be included in Table 1, as it also directly addresses brine migration in the Mount Simon.

AC (Page 5705) Line 3: We have performed two extra simulations considering a linear salinity gradient in addition to the scenarios with sharp salt-/freshwater interface. The additional results will be presented and discussed in the manuscript. Line 11: sentence

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will be revised. Line 13: The beginning of the sentence will be deleted. The difference between deep aquifers in sedimentary basins, which are generally saltwater-bearing and the shallow aquifers that can represent considerable freshwater resources will be made clearer. Line 14: sentence will be revised (see above). Line 14: The reservoir (Detfurth Fm) in our model is the saline aquifer, which contains brine. The uppermost aquifer in the model, at a depth of about 100 m in average, is the Rupelian basal sand, which is also saltwater-bearing, however with significantly lower salt concentrations. The top of the Rupelian basal sands mark the saltwater-freshwater boundary in the investigated area, which lies at a depth of 100 m below mean sea level, in average (Stackebrandt and Manhenke, 2004For simplification, we assume that the Rupelian basal sands contain freshwater in the present study. All freshwater units in our model are termed as "shallow" (Rupelian basal sands), whereas the saline aquifers are referred to as "deep". We will explain this more precisely in the manuscript. Line 20: Four references will be added to the manuscript (Dempsey et al., 2014; Fitts and Peters, 2013; Chiaramonte et al., 2008; IEAGHG, 2008; Bense and Person, 2006; Forster and Evans, 1991). Line 25: The publication of Person et al. (2010) will be integrated into Table 1 as well.

RC (Page 5706) Line 2: delete "thereby" Line 2: I am not aware how different initial conditions impacted the pressure results in the two studies. The main difference was the choice of rock compressibility and different representation of compressibility in the two simulators. The authors need to be more precise. Lines 11-12: "whether brine is allowed to spread laterally in the upper aquifer" If the brine can't flow then it is not much of an aquifer, so I don't know what this statement means. Lines 23-24: This is a strange statement. I would expect that a low permeability fault will allow very little flow into an overlying aquifer. Delete or explain. Line 29: "should avoid" sounds like the convergence was not tested. Either clearly state it was tested and convergence was reached, or state the opposite and devalue the results of the numerical model in the paper.

AC (Page 5706) Line 2: "Thereby" deleted. Line 2: The different assumptions made in Person et al. (2010) and Zhou et al. (2010) primarily concern formation permeability, formation compressibility, boundary conditions, distribution of injection wells and dimension of simulations. We will add the main differences to the manuscript. Lines 11-12: We will clarify, that brine flow behavior in the upper aquifer depends on the lateral extent of this aquifer, if brine is allowed to spread unhindered or whether barriers to flow exist due to low-permeability layers or impermeable fault zones in that aquifer, limiting lateral brine propagation. Lines 23-24: It will be mentioned which fault permeabilities were investigated in Tillner et al., 2013 and that these did not result in a significant different degree in shallower aquifer salinization. Line 29: It will be stated clearly that the simplifications in our model significantly improved the convergence efficiency of the simulations and that we did not observed any numerical artefacts.

RC (Page 5707) Line 5: "general understanding of underlying processes" It would seem that the underlying processes (i.e., single phase flow in a porous medium) are pretty well understood at this time. Line 8: I'm a little surprised by this very detailed description of the geology. The goals of the paper stated in the previous paragraph don't include site specific conclusions. In the end, a very simple model is used. I would delete this section as it distracts from the paper.

AC (Page 5707) Line 5: We are indeed only looking at pressure driven single phase flow. However, as shown by the results, the course of the four fault zones and the hydraulically conductive fault length impacts fluid flow out of the fault in the shallow aquifer and thus pressure gradients (Figure 4). We will delete "general understanding of underlying processes" and explain the effects mentioned above more detailed. Line 8: Chapter will be shortened significantly. Only the layers and faults integrated into the geological model and their main characteristics will be introduced in a brief description of the geology.

RC (Page 5709) Line 20: Why is the caprock permeability assumed lower than in the previous study? Are there additional measurements? Explain. Line 25-27: I would

describe the different scenarios before this.

AC (Page 5709) Line 20: In a previous study, Kühn and Kempka (2015) investigated the impact of CO2 storage in saline aquifers by upward brine migration through a sequence of caprocks and showed that saltwater does not reach into the groundwater resources through intact caprocks with a permeability of at least 10-17 m2. In the present study, the caprock above the storage formation mainly consists of marine evaporates such as anhydrite and halite. An intact anhydrite or halite is most likely characterized by permeabilities lower than 10-17 m2, preventing salinization of overlying units according to the authors mentioned above. From our point of view, brine migration through the caprock sequence is rather unlikely due to the lithology on site and we therefore defined the caprocks as impermeable. This will be explained clearer now in the manuscript. Line 25-27: We are convinced that the chosen set of scenarios is easier to follow if the applied geological model and its setup is described at first (e.g. layer structure, fault damage zone volume, location of faults, distance to injection well etc.). Therefore, we keep the chapter sequence as it is in this part.

RC (Page 5710) Lines 8-10: What is the displacement at the faults studied here? Without that information, the whole discussion of 250m fault width is not useful. Line 17: I would describe the fault scenarios earlier, so that you can point to the 2 km fault opening here as well and reference it in figure 1b.

AC (Page 5710) Lines 8-10: displacements at the faults range between several hundred meters up to 1,000 m (as described in chapter 2 – study area). We have added this information to the manuscript. Line 17: see answer comment above (Page 579, Line 25-27).

RC (Page 5711) Line 2: ". . . to be between those of. . ." Line 4: Otherwise there wouldn't be time dependent flow patterns? Line 9: ". . . first and last. . ." Line 9-10: Why? Line 13 and 16: why the two different volume multipliers? Aren't both constant pressure boundaries? I'm not sure that the volume modifiers have to be mentioned at all, as

they are just a quirk of how TOUGH2 represents boundaries. But these are not quasi-infinite boundary conditions, as far as I know. These massive-volume cells will keep pressure pretty much constant, while in a quasi-infinite boundary the pressure should be able to increase. Explain. Line 21: Strange sentence: initial conditions are defined at a single point in time; the initial conditions are based on a geothermal gradient, so not constant in space. Authors need to be more precise in their writing. Line 28: not sure how the visualization is relevant here. Doesn't seem to be used in any figure.

AC (Page 5711) Line 2: mistake will be corrected as commented by referee. Line 4: "time dependent flow patterns" will be deleted. Line 9: comment adopted. Line 9-10: Brine migration across the faults is indeed possible since no impermeable fault core was considered, however, by application of a higher fault than reservoir permeability, brine migration occurs almost solely upward into the overlying formations and is negligible in horizontal direction across the faults (in Detfurth and Muschelkalk formations). This will be explained more precisely in the manuscript. Line 13 and 16: The higher volume multiplication at the boundary elements of the Tertiary Rupelian basal sands is based on the assumption that a continuous hydraulic connection throughout the formation is more likely in the younger and less consolidated sedimentary deposits than in the more tectonically influenced deeper rocks. Pressure at the boundary of the Rupelian remains constant during the simulations (infinite aquifer), whereas in the reservoir an increase below 0.1 bar was observed in the open or quasi-infinite case. Line 21: will be changed to "initial temperature distribution remains constant in time and space" Line 28: statement will be deleted as commented by referee.

RC (Page 5712) Line 1-2: all models are run for hydrostatic conditions. Do you mean hydrostatic initial conditions? Line 6: I'm missing a reason why the authors didn't use CO_2 for injection as this is a study of CO_2 sequestration site. Is it just the computational expense? 1.8×10^6 elements for 20 years doesn't seem intractable on a 256 processor machine. Line 12: the density "sums up"; strange terminology Line 16: why "while"? Line 21-25: this is too long to just say that diffusion is irrelevant for the problem

considered here.

AC (Page 5712) Line 1-2: will be corrected to "All simulations start from hydrostatic pressure conditions". Line 6: The reason why we did not use CO2 injection will be explained more clearly. It was planned to inject CO2 into the Lower Mesozoic formations at the top of an anticline structure located at a distance of about 4.5 km from the nearest fault zone. We use the same injection well location in the present study, however, since we are focusing mainly on the long-term effect of brine displacement, it is likely that without topographic variations and structural trapping below an e.g. anticline, CO2 reaches the fault zone after a couple of years. This would make our simplified model more complicated as intended, so we decided to inject brine. We are aware of CO2 compressibility effects and that the displaced volume of brine might be smaller when injecting CO2, however we believe that compressibility effects are negligible in the long-term after the injection stop when pressure comes to equilibrium, as also demonstrated by Nicot, 2008. Line 12: corrected to "Taking into account the salinity of 25 %, brine density is 1 175 kg m 3". Line 16: sentence will be revised: "brine densities are calculated in TOUGH2-MP/ECO2N for each element during the simulation and fluid compressibility is then considered by its density changes". Line 21-25: we will shorten this section as recommended by referee.

RC (Page 5713) Line 6: I really like the system of identifying the different scenarios. Line 17: It would be interesting to which processes the authors are referring to.

AC (Page 5713) Line 17: We will be more precise: These settings represent three baseline cases, which should primarily demonstrate the impact of effective damage zone volume and different courses of the fault zone on the degree of upper aquifer salinization and salinity distribution, respectively. As mentioned earlier, the course of the four fault zones and the hydraulically conductive fault length/ effective damage zone volume impacts fluid flow out of the fault in the shallow aquifer and thus pressure gradients.

RC (Page 5714) Line 1: this result is not surprising for the close boundary case. For a closed incompressible domain all the pressure relief comes from brine flowing up the fault, so that the same mass will reach the freshwater aquifer. However, in an open domain, most of the pressure relief will come from horizontal brine migration in the injection formation. In that case, fault permeability should make a difference as the duration of the increased pressure is independent of fault permeability. In addition, I don't think that retardation should be neglected completely as regional groundwater flow may be enough to dilute in the incoming high salinity formation brine. Line 6: is this a result from a previous study or a result of this study? Either cite the previous study in the text and figure 3 or move to results section. Alternatively, you could describe these as "initial" or "preliminary" results, but then you need to delete figure 3 and reduce the level of detail in discussion here. Line 16: mass flow of what? Brine? Salt? Ideally it would be salt, but for comparisons between different scenarios brine flow rate would be fine, as salinity is constant. Line 25: more flow into parts facing the injection than parts not facing the injection. Why is brine flowing into the fault from the side not facing the injection? Is brine flowing around the faults or is this brine being drawn in from the boundary? The arrows in the plot in figure 4 (lower left) both point from the same side, so no help in explaining there. What are the colors/size of dots and background color mean in the two left plots? Where is the brine going that is entering the fault, but not leaving it at the top (i.e., more flow at the bottom than at the top)? Is this all compressibility?

AC (Page 5714) Line 1: We totally agree with the referee that in an open domain, most of the pressure relief comes from horizontal brine migration in the injection formation. Consequently, less brine is displaced into up the fault. We therefore decided to investigate only the temporal effect on upward brine migration for different fault permeabilities and closed reservoir boundaries, since the results by Tillner et al. (2013) have shown that even for a number of fault with very high permeabilities (and closed lateral reservoir boundaries), the relative mass change of water and salt in the uppermost aquifer was relatively small. Line 6: The retardation in mass flow for different fault permeabilities

and closed boundaries was already observed in previous simulations. We decided to show this effect by three different simulations with fault permeabilites of 700 mD, 200 mD and 10 mD (figure 3) but in our scenario analysis considering different boundary conditions, fault length and the presence of an overlying reservoir, the fault permeability remains with 700 mD. This is obviously not clear in the manuscript. We will revise this part and delete the information on previous studies (not published) which are indeed misleading for the reader. Line 16: What is meant is brine mass flow. Missing information will be added to the manuscript. Line 25: In the reservoir, brine is displaced mainly into parts of the undulating fault located closer to the injection point. In the shallow aquifer and in case of four open faults, brine that flows out of the faults migrates into the Mittenwalde Block (compartment in the central model domain bounded by the four fault zones; Figure 1) and towards the open model boundaries. Consequently, pressure gradients are becoming lower in the Mittenwalde Block over time so that flow out of all faults towards the lateral boundaries dominates at the final injection stage (most noticeable for Fault 3; Figure 4). We will edit Figure 4 since the colors are not clear enough.

RC (Page 5715) Line 1: why is brine not exiting the fault symmetrically? The flow rates are so low, that pressure interference in the upper aquifer would be surprising. Why are there different pressures? Line 6: farther Lines 5-6: Why would salinity be higher farther away from the injection? I think I am misunderstanding the sentence. Line 23: this backflow is surprising. The small increase in density is enough to work against the dissipating pressure gradient, I guess. I think this backflow is somewhat over stated, as mixing from local recharge and regional flow probably will have a strong effect over a 400 yr time period. In figure 5 the white arrow down is as big as the one coming up which gives the impression that the rates are comparable. I realize that the arrows are for direction only, but I would makes them different thicknesses.

AC (Page 5715) Line 1 and Lines 5-6: See above. In the shallow aquifer and in case of four open faults, brine that flows out of the faults migrates into the Mittenwalde Block

(compartment in the central model domain bounded by the four fault zones; Figure 1) and towards the open model boundaries. Consequently, pressure gradients are becoming lower in the Mittenwalde Block so that flow out of all faults towards the lateral boundaries dominates at the final injection stage (most noticeable for Fault 3; Figure 4). Thus, after 20 years of injection, salinity increase is slightly higher e.g. west of fault 3 than in the eastern part. In addition, the course of the faults affects the direction of brine flow out of the fault and thus pressure gradients. This might explain why we do not see a symmetric distribution of brine along the faults (primarily fault 1). We will explain this more clearly in the revised manuscript and will add values accordingly. Line 6: mistake will be corrected. Line 23: We will add the pressure difference at the time of brine backflow and rates to the manuscript.

RC (Page 5716) Lines 2-6: I think it is obvious that the flow distances will be different for locations with different pressures, so I would not mention that. However, I think it is very powerful to state, as the authors do, that flow into the freshwater aquifer only occurs from the upper part of the fault. At first reading, I was a little confused about where the authors were counting from, so I would suggest that the authors stress that they are counting from the bottom of the freshwater aquifer. Line 14: shouldn't this be "fault" not "faults" as only one fault is active in this scenario. If I understood the setup correctly, then the other three faults and the inactive parts of fault one are "inactive". In my experience, inactive elements in TOUGH2 have constant values, so they should keep the initial pressure. From figure 6a I don't see any pressure for fault three (as stated in the text). Am I reading the text of the figure wrong? In figure 6a there is not legend for the three lines. I'm assuming it is the same as in figure 6b. Needs to be stated directly. Also in figure 6a: for the short fault, why is the pressure behind the fault increasing? Is the brine flowing through the inactive part of the fault? Line 20: I think this makes a lot of sense, as the injection is right next to fault one.

AC (Page 5716) Lines 2-6: Yes, we are counting from the bottom of the Rupelian basal sands. We will add this information to the manuscript. As commented by the referee

we will delete the part where we explain the different flow distances for locations with different pressures. Line 14: Yes, this should be "fault" and not "faults". Mistake will be corrected. In TOUGH2 cells with a cell volume of 0 pose Dirichlet boundary conditions. In order to avoid misunderstanding we will delete the term "inactive" and state that the elements of the impermeable fault zones are simply not considered in the model grid. Line 20: If this is too obvious, we can delete this information.

RC (Page 5717) Line 5: I think this undersells the time-scales involved. Mixing in the freshwater aquifer might make the salinity influx unnoticeable over 300 yr period. Line 14: why is there residual freshwater? This is a single phase simulation, so no residuals. I don't see how the density makes a differences for horizontal flow? Line 21: Didn't this already get discussed earlier?

AC (Page 5717) Line 5: We will mention this effect in the manuscript. Line 14: What the authors mean is the "remaining" freshwater. Residual will be deleted. The density might not make a difference for horizontal flow. We will consider this comment in the revised manuscript. Line 21: We will delete this sentence.

RC (Page 5718) Line 8: Setting the boundary conditions to constant pressure will not allow the pressure to increase at the boundary. I don't think this needs to be stated.

AC (Page 5718) Line 8: We will delete this sentence.

RC (Page 1519) Lines 1-2: all of these statements would be more meaningful in terms of mass of salt. Again, the time scale is important here. 1500 yrs is a long time. Line 3: I didn't read section 5.3 in detail, as the listing of results is becoming tedious and I'm losing sight of the goal of the paper. In my opinion the entire results section needs to be shortened.

AC (Page 1519) Lines 1-2: We will add the mass of salt flowing back into the fault and emphasize the time scale at this point. Line 3: We totally agree with the referee and we will significantly shorten this section in the revised version.

RC (Page 5721) Line 23: "only" is twice in this sentence

AC (Page 5721) Line 23: we will correct this mistake.

RC (Page 5722) Line 15-16: I find this to be a very strong statement. What are the relevant processes other than flow? Line 18: What else than a pressure increase in the injection formation could be a driving factor? Brine is more buoyant than freshwater, so gravity is not a driving factor. What else is there? Lines 23-24: it seems that this is the first time that "effective damage zone volume" is mentioned, other than in the title. Title needs to be changed. Pinning this on volume is strange, as the authors assume a fixed width and only vary length.

AC (Page 5722) Line 15-16: The courses of the faults and the compartmentalization in the central model domain due to the four fault zones that enclose this compartment are affecting flow. This is indeed not a process. We will correct that. Line 18: We agree. This sentence will be revised. Lines 23-24: We have added the effective damage zone volumes for the three different fault length to chapter 4 (set of scenarios). The fault element volume can be derived from TOUGH2, the effective porosity is known as well.

RC (Page 5723) Line 10: This entire paragraph's message is that the choice of boundary conditions is important (open vs closed). Not much of a discussion.

AC (Page 5723) Line 10: Comment will be considered. We totally agree with the referee and will revise the main parts of the discussion.

RC (Page 5724) Line 4: what does "effective volume of the hydraulically conductive length of the fault zones" mean. Length and volume? Line 9: more interesting would be total area. Line 11: "impermeable" would mean that no flow crosses them in the injection formation. This is not shown by the results. The authors need to be more precise. Lines 10-12: Location of salinization is pre-determined. I would think that is obvious. Brine is going to leak at the faults, no? Line 15: so was width as far as I can tell

AC (Page 5724) Line 4: This is indeed a mistake. Either hydraulically conductive fault length or effective damage zone volume. We will correct that. Line 9: We will add the total area affected by salinization to the revised manuscript. Line 11: It will be clarified that the faults do not intersect the injection formation. Lines 10-12: If this is too obvious, we can delete this information. Line 15: This is true. The sentence will be revised to make this clear.

RC (Page 5725) Line 11: How about the Birkholzer et al (2011) "Brine flow up a well caused by pressure perturbation from geologic carbon sequestration - static and dynamic evaluations" paper?

AC (Page 5725) Line 11: We will discuss the publication from 2011 as well.

RC (Page 5726)

Line 13: it seems the only site-specific insights are that there are more intermediate layers and that the salinity distribution is known. Why not run a model with the known salinity distribution then? Line 25: but only if they have open boundaries, right?

AC (Page 5726) Line 13: As stated previously we have perfomed two extra simulations considering a linear salinity gradient in addition to the scenarios with sharp salt-/freshwater interface. The additional results will be presented and discussed in the manuscript. Line 25: Yes. Missing information will be discussed.

RC (Page 5727) Lines 12-21: I would structure this differently. I would first compare closed to open and then mention the impact of different fault lengths and existence of intermediate aquifer. Line 28: I would make the argument that the larger fault length (and thus more leakage area) leads to lower pressures which leads to less flow which leads to a shallower depth from which leakage is occurring. This gives more or less the same information as written, but in a more logical sequence (at least for me).

AC (Page 5727) Lines 12-21: We will consider this in the revised manuscript. Line 28: We totally agree. The proposed sequence is more logical and we will adopt it in our

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RC (Page 5728) Line 2: "very permeable" faults are not discussed in this paper, so should be deleted here Line 4: the entire length of a fault is affected by displacement, so sentence needs to be rewritten Line 10: the term "damage zone volume" is used almost exclusively in this section when the authors really tested different lengths, not volumes. This may sound like semantics, but I would expect a very thin long fault to act differently than wide short one. Line 13: the mention of geomechanics seems out of place here. Maybe the discussion section would be a better fit. Lines 20-21: I think this is a difficult statement to make as the validity of the modeling results is not tested in any way. Are there processes that might be important that are not represented here? Is the fault structure (highly permeable damage zone without low permeability fault core) a sufficient description? Does a one element wide fault correctly represent flow in and out of the fault zone?

AC (Page 5728) Line 2: From our point of view, 700 mD is very permeable, at least for a fault zone. Line 4: This is true. The mistake will be corrected. Line 10: We have added the effective damage zone volumes for the three different fault length to chapter 4 (set of scenarios). The impact of different fault structures (e.g. very thin long fault vs. wide short one) on the (expected) fluid flow behavior can be mentioned in the discussion. Line 13: We agree and will consider it in the revised manuscript. Lines 20-21: We will emphasize that different simplifications and assumptions have been made and agree with the referee that the assumptions made in our study are only valid for certain faults. Brine migration across the faults is indeed possible since no impermeable fault core was considered, however, by application of a higher fault than reservoir permeability, brine migration occurs almost solely upward into the overlying formations and is negligible in horizontal direction across the faults (in Detfurth and Muschelkalk formations). This conservative approach represents a least favorable scenario for upper aquifer salinization. Further research is underway to extend the assumptions made by the implementation of heterogeneous fault zones with spatial variations in porosity and

permeability and related non-uniform architecture and fault inclination. Nonetheless, we will include a discussion on the high complexity of faults.

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