Review History for "Far-field modelling of THM processes in rock salt formations"

Florian Zill, Christian B. Silbermann, Tobias Meisel, Fabiano Magri, Thomas Nagel
2023

Summary (optional)

The paper was sent to three reviewers — Reviewer A, Dr. Ayman Abed (Reviewer B) and Reviewer C. The reviewers remained anonymous during the entire review process and the authors were anonymous for the reviewers. After the reviewing process was complete, reviewer B agreed to disclose his identity. In Review Round 1, the reviewers provided a series of comments for the authors and required a revision of the manuscript. In Review Round 2, the reviewers recommended the manuscript for publication.

Review Round 1

Reviewer 1 (anonymous)

The authors wrote a good paper, where the content of the paper is explained in a very clear and understandable way. Figures are also given a good quality. As a reviewer, I have only some smaller comments that lead to some minor revisions:

1. In line 116, there is a small layout error, because the word "post-processing" exceeds the length of the line.
2. In line 155, there is a doubled "the".
3. In line 336, a figure number is not correctly referenced. There is only "??" given.
4. After each equation, the next line should start left-aligned, because it is not really a new paragraph there. It just continues the text from before the included equation. 507–521.

Reviewer 2 (Ayman Abed)

Overview and general recommendation:

The paper presents an interesting large-scale simulation of the effect of glaciation on geological formations. The simulation includes different THM couplings and employs a special viscoplastic material model to account for the creep effect of the so-called rock salt strata. The main trigger behind the study is to provide a means to evaluate the safety of storing nuclear waste in rock salt as a host rock for 1 million years under glacial cycles.

The paper is well-written, structured and easy to follow. For the scientific content, I found the contribution interesting for researchers working on Multiphysics and nuclear waste management and thus relevant to the readers of Open Geomechanics. However, I am afraid that the authors have assumed, in several places in the text, that the reader already has some background about the concept they are dealing with. Thus, before recommending the paper for publication, I would like the authors to address the following comments/questions in their revised version:

- Line 13: You stated: 'Thus, the effect of glacial cycles on potential deep geological repositories (DGR) in rock salt has to be investigated'. The effect on deep geological repositories; in what sense? Could you be specific?
- Line 37: 'highly sensitive to differential stresses'. What do you mean by 'differential stresses'?
- Line 35-45: It would be helpful to provide a figure/sketch clarifying the terms 'crystal lattice', 'dislocation', 'grain boundaries', 'fluid phase', 'inclusions'.
- Line 66: 'Hydraulic tightness can therefore be assessed on the basis of integrity criteria.'. What do you mean by 'integrity criteria'? Could you elaborate more on what you mean by 'integrity criteria', 'fluid pressure criterion' and 'dilatancy criterion' besides what is given in the Appendix. Why does one need to check against these criteria? Maybe you want to put that in the context of the design process.
- Line 76: 'For the theoretical background of the THM coupled FEM formulation used in this study, we refer to Wang et al. [2021].'. It would be good if you could introduce the employed governing equations, that would make it much easier for the reader when analysing the results.
- Line 91: 'Ensuring consistency of the results both from a physical and a numerical point of view is therefore often a cumbersome task for modellers.'. Could you explain what you mean by this sentence?
- Could you provide more information on the used finite element type, total number of elements, average element size and the effect of mesh and time-stepping refinement on the results?
- 'To avoid a numerically undesirable jump in values, for 200 m in front of the glacier, the temperature is interpolated with a smooth step function'. Could you show this function?
- 'A conservative proxy model "DWR-Mix 89/11" as described in the GRS RESUS reports [Bertrams et al., 2020]' Could you introduce and explain the model in detail? It is fundamental to make the section 'Repository source term' understandable.
- Could you define 'the von-Mises equivalent stress' in terms of principal stresses? Why did you choose this stress measure? Are you employing any failure criterion when modelling the rock salt?
- Could you explain Eq. 5?
- Line 336: Fix '?? displays'.
- Line 423: You stated: 'However, as the glacier begins to retreat, the direction of creep reverses and there is a partial reduction in the accumulated displacement'. Is it the reversal of creep or simply because of the unloading effect?
- Line 456: You stated: 'Large-scale models are a fundamental tool for the assessment of the long-term stability, integrity and safety of salt formations in a wide range of engineering applications'. While I agree with this statement, I could not find any reflection in your paper on that. For example, is it safe? Is it stable? Why? How did you judge?
- Line 461: 'the automation of simulation workflows [Lehmann et al., 2024]': It would be good to include brief text on this automation.
- Line 475: 'mixing Robin and Neumann types': To me, Robin's boundary condition is already a mixed boundary condition (Dirichlet+Neumann).
- In the abstract, you stated, 'The rock salt creep law, applied over the extensive timescales at hand, approached the limits of the finite element-method (FEM) with small-strain assumptions.' In which sense and what do you mean by that?

Reviewer 3 (anonymous)

This paper is about a THM model study based on a generic model of a stratiform salt formation.

In general, the paper is well-written, scientific sound and worth to be published.

A general characteristic of the paper is that it is quite comprehensive. I am fine with this; however, as a consequence several topics are only very briefly or not at all explained.

Some detailed remarks:

Chapter 2.1: first it is stated that the 3D model is simplified for performance reasons; however, then it is said that only 2D cross sections are used for the modeling. For me this is not logic, if only 2D sections are used, why was it necessary to simplify the geology?

Line 140 or where ever it fits: please give number of nodes and elements of the model

Line 163: you may want to consider a reference to https://doi.org/10.1016/j.cageo.2014.03.001 as it is somewhat newer and also used this approach.

Equation 3: the parameter beta_p is not explained

Line 192: which four radionuclides where used?

Line 223: 'BGRa' – meaning??

Line 276: why mention other (better?) methods, when not used? I suggest deleting this sentence.

Chapter 2.8 how are the THM equations solved? Monolithic or coupled by the Newton method? This is not clear to me.

Line 327: although this is stated at the very end of the paper it should be discussed already here: when using a 2D model its extension in the 3rd direction is 1 m. Therefore the volume considered for the heat source is not realistic. The real occurring temperatures are certainly lower. This should be made very clear. Generally this approach is quite questionable. It would have been better to derive temperatures based on a 3D model occurring within the repository and use these temperatures as time dependent BC instead the heat source. BTW – the temperature given violates the maximum temperature of 100 °C allowed by the StandAG – however BGE increased this value recently to 150 °C.

Line 336: '??'

Line 340: this uplift is a consequence of the values for the thermal expansion not discussed at all and not referenced in the final table. A little bit more of information would be good.

Line 475: this is speculative – suggest deletion.

Line 487 – 488: speculative – suggest deletion.

Line 491: why is it advisable to use a plastic material law for the overburden rocks? Why is the elastic approach not valid? In my opinion elasticity is for these kind of rocks an okay presumption.

Line 555: in http://www.sciencedirect.com/science/article/pii/S1876610215016422 and https://www.sciencedirect.com/science/article/pii/S0309170817307510 approaches are shown to model the movement of the freezing (thawing) front using an adaptive mesh refinement. Such an approach should at least be mentioned as it helps a lot by mitigating the mentioned numerical problems.

Line 570: 'the following figures' – which?

Table 5: why is the Biot coefficient for Buntsandstein 0.5 while it is 0.6 for the remaining rocks. To my knowledge it is very challenging to obtain valid Biot coefficients. Literature typically refers to 0.6. For conversativity also 1 might be suitable.

Final general remarks:

Lack of phase change: it is indeed a short-coming of this study that the significant decrease of hydraulic conductivity due to to phase change is not considered. Actually it wouldn't have been too difficult to set K to a value say 1E-6 times smaller in case T < 0 °C.

Model philosophy: performance vs. accuracy: this is mentioned several times in the paper for justification of model simplifications – i.e. they are necessary for performance reasons. However, it remains somewhat unclear which decrease of performance is meant. When is performance decrease relevant enough for justifying relevant model simplifications?

Finally:

- have there been any mesh convergence studies?
- Quite often sensitivity studies are part of such model studies (I don't say that they are always relevant) – is there a reason this is missing here?

Author Response

We are very grateful for the time the reviewers have taken to provide their extensive and constructive feedback. The reviewers comments have significantly improved our manuscript. We have carefully revised our work following their suggestions and we now kindly request to consider the revised version for publication approval.

Additionally to the reviewers remarks, we rediscretized our model with quadratic elements (Tri6), to mitigate some minor locking artefacts and replaced all figures accordingly. The results are qualitatively almost identical as before and the conclusions remain the same.

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Responses to the Reviewer A:

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The authors wrote a good paper, where the content of the paper is explained in a very clear and understandable way. Figures are also given a good quality. As a reviewer, I have only some smaller comments that lead to some minor revisions:

In line 116, there is a small layout error, because the word "postprocessing" exceeds the length of the line.

Thank you for noticing.
action: We fixed the layout error.

In line 155, there is a doubled "the".

True, Thank you.
action: We removed on instance of "the".

In line 336, a figure number is not correctly referenced. There is only "??" given.

Thanks for pointing this out.
action: We fixed the figure reference.

After each equation, the next line should start left-aligned, because it is not really a new paragraph there. It just continues the text from before the included equation.

Agreed.
action: We removed the indentation after equations.

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Responses to the Reviewer B:

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The paper presents an interesting large-scale simulation of the effect of glaciation on geological formations. The simulation includes different THM couplings and employs a special viscoplastic material model to account for the creep effect of the so-called rock salt strata. The main trigger behind the study is to provide a means to evaluate the safety of storing nuclear waste in rock salt as a host rock for 1 million years under glacial cycles. The paper is well-written, structured and easy to follow. For the scientific content, I found the contribution interesting for researchers working on Multiphysics and nuclear waste management and thus relevant to the readers of Open Geomechanics. However, I am afraid that the authors have assumed, in several places in the text, that the reader already has some background about the concept they are dealing with. Thus, before recommending the paper for publication, I would like the authors to address the following comments/questions in their revised version:

Line 13: You stated: 'Thus, the effect of glacial cycles on potential deep geological repositories (DGR) in rock salt has to be investigated'. The effect on deep geological repositories; in what sense? Could you be specific?

These processes can significantly impact the mechanical and hydraulic properties of the host rock, including the development of secondary porosity and permeability. These events could compromise the effectiveness of the DGR.
action: Specified further in text.

Line 37: 'highly sensitive to differential stresses'. What do you mean by 'differential stresses'?

The term differential stresses is sometimes used in the context of triaxial testing, where they coincide with a certain deviatoric metric.
action: We rephrased to the more general term deviatoric stresses as it is a more comprehensive descriptor in the study of viscoplastic/viscoelastic material behavior under multi-axial stress states.

Line 35-45: It would be helpful to provide a figure/sketch clarifying the terms 'crystal lattice', 'dislocation', 'grain boundaries', 'fluid phase', 'inclusions'.

These concepts underpin the general understanding of the employed models. We do explicitly work at the grain scale in our study but mention the concepts to provide a microstructural motivation for the chosen constitutive approach.
action: We added a figure to illustrate the terms.

Line 66: 'Hydraulic tightness can therefore be assessed on the basis of integrity criteria.'. What do you mean by 'integrity criteria'? Could you elaborate more on what you mean by 'integrity criteria', 'fluid pressure criterion' and 'dilatancy criterion' besides what is given in the Appendix. Why does one need to check against these criteria? Maybe you want to put that in the context of the design process.

The term 'integrity' here implies that the properties of the geological barrier which ensure the safe containment of the waste remain intact. It has been experimentally established that certain mechanical, hydraulic or thermal effects can cause the appearance of secondary porosity and permeability by, e.g., dilatant deformation or pore pressure exceeding tensile strength measures. Actually, these criteria are fundamental to assess how these effects could compromise barrier function. Therefore, barrier integrity criteria have been established that allow engineers to assess the extent to which prevailing loads and stress states comply with barrier integrity requirements.
action: Added explanation to text. We also pointed the reader to further references. The DGGT will soon publish a book in which these concepts are explained in detail. Unfortunately, we cannot cite that, yet.

Line 76: 'For the theoretical background of the THM coupled FEM formulation used in this study, we refer to Wang et al. [2021].'. It would be good if you could introduce the employed governing equations, that would make it much easier for the reader when analysing the results.

Agreed.
action: We added a section for the governing equations.

Line 91: 'Ensuring consistency of the results both from a physical and a numerical point of view is therefore often a cumbersome task for modellers.'. Could you explain what you mean by this sentence?

Physical models are complex and need to be thoroughly verified when implemented in code. Validation against experiments is, in this field, done in large international initiatives and can take a very long time. From a numerical point of view, element quality, convergence of the discretization, stability, artifacts etc. need to be checked. For large 3D models with complex

geometries, this can become prohibitively expensive, considering also, but not only, the workload of meshing.
action: None.

Could you provide more information on the used finite element type, total number of elements, average element size and the effect of mesh and time-stepping refinement on the results?

Certainly.
action: We added more information in the section "Numerical settings" and added a section regarding the convergence behavior to the appendix. Note, that the results in this revised version are simulated on tri6 elements. The initial manuscript was on quad4 elements and both provide similar results.

'To avoid a numerically undesirable jump in values, for 200 m in front of the glacier, the temperature is interpolated with a smooth step function'. Could you show this function?

Sure.
action: We added the function to the text.

'A conservative proxy model "DWR-Mix 89/11" as described in the GRS RESUS reports [Bertrams et al., 2020]' Could you introduce and explain the model in detail? It is fundamental to make the section 'Repository source term' understandable.

The model is what is already explained in detail in Section 2.3.
action: None.

Could you define 'the von-Mises equivalent stress' in terms of principal stresses? Why did you choose this stress measure? Are you employing any failure criterion when modelling the rock salt?

This is a commonly used scalar measure for deviatoric stress widely used in the salt literature. It is a convenient metric for evaluating the stress state without introducing unnecessary complexity. No failure criterion was used in the simulation. The employed integrity criteria check the stress results for failure.
action: The equation was added.

Could you explain Eq. 5?

The model is quite complex and we have to keep aspects short that can be considered standard in the field. We added a few more explanations but refer to the mentioned references for further details.
action: We added some more explaination to equation 5.

Line 336: Fix '?? displays'.

Thanks for pointing this out.
action: We fixed the figure reference.

Line 423: You stated: 'However, as the glacier begins to retreat, the direction of creep reverses and there is a partial reduction in the accumulated displacement'. Is it the reversal of creep or simply because of the unloading effect?

The phenomenon observed is indeed reversed creep because the material continues to deform in the opposite direction even after the glacial load has been fully removed. This behavior is consistent with the viscoplastic nature of rock salt. Our model captures this time-dependent response.
action: None

Line 456: You stated: 'Large-scale models are a fundamental tool for the assessment of the long-term stability, integrity and safety of salt formations in a wide range of engineering applications'. While I agree with this statement, I could not find any reflection in your paper on that. For example, is it safe? Is it stable? Why? How did you judge?

We understand the reviewer's wish but have to be careful at this stage not to draw specific conclusions bases on a generic model that, despite being complex, still lacks features relevant in glacial cycles. The motivation of the study is to provide simulation technology that facilitates such analyses and to demonstrate how certain physical effects, some of which have only recently been recognized, contribute to THM behaviour under glacial loads. We can observe what the integrity criteria do under the present conditions and draw limited conclusions in this regard.
action: We elaborated further in the section "Evaluation of integrity criteria´´.

Line 461: 'the automation of simulation workflows [Lehmann et al., 2024]': It would be good to include brief text on this automation.

Agreed.
action: Added a bit more context for automated simulation workflows.

Line 475: 'mixing Robin and Neumann types': To me, Robin's boundary condition is already a mixed boundary condition (Dirichlet+Neumann).

Indeed, this was meant as Robin BC on one lateral boundary, Neumann BC on the other lateral boundary.
action: This was considered speculative and thus was removed.

In the abstract, you stated, 'The rock salt creep law, applied over the extensive timescales at hand, approached the limits of the finite element-method (FEM) with small-strain assumptions.' In which sense and what do you mean by that?

By that time deformations had accumulated that exceeded 10 %. We made some comparison simulations with finite strain formulations in a pure mechanical setting and the results were not affected qualitatively. The small strain assumption is thus questionable from a formal point of view, but the simulation results presented are still valid.
action: None.

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Responses to the Reviewer C

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This paper is about a THM model study based on a generic model of a stratiform salt formation. In general, the paper is well-written, scientific sound and worth to be published. A general characteristic of the paper is that it is quite comprehensive. I am fine with this; however, as a consequence several topics are only very briefly or not at all explained.

Chapter 2.1: first it is stated that the 3D model is simplified for performance reasons; however, then it is said that only 2D cross sections are used for the modeling. For me this is not logic, if only 2D sections are used, why was it necessary to simplify the geology?

We agree that our initial phrasing was unclear. While some geometric complexity is reduced (simplified), this workflow allowed to balance accuracy with computational feasibility, given the large scale and long-term nature of the simulations. Despite these simplifications, the key physical processes are preserved, and the results are qualitatively consistent with more detailed 3D models.
action: Reworded.

Line 140 or where ever it fits: please give number of nodes and elements of the model

Done.
action: We added the numbers.

Line 163: you may want to consider a reference to https://doi.org/10.1016/j.cageo.2014.03.001 as it is somewhat newer and also used this approach.

Agreed.
action: We added this reference.

Equation 3: the parameter β_p is not explained.

It is indeed missing in text.
action: We added the parameter explanation.

Line 192: which four radionuclides where used?

From our understanding of the Resus report, the leading nuclides are artificial / virtual. They are calculated such, that they provide an optimal fit to a more computationally expensive decay simulation.
action: We changed it to "four artificial leading nuclides"

Line 223: 'BGRa' – meaning??

The BGRa model is a simple stationary creep model developed at Bundesanstalt für Geowissenschaften und Rohstoffe and a common reference model. It is also linked to the creep classes of rock salt.

action: We rephrased it to "the stationary creep model called BGRa"

Line 276: why mention other (better?) methods, when not used? I suggest deleting this sentence.

It was meant to inform the reader that there are arguably better methods available, that are unfortunately not included in this study due to limited time and the complexity of implementation.
action: We deleted the sentence.

Chapter 2.8 how are the THM equations solved? Monolithic or coupled by the Newton method? This is not clear to me.

We utilized a monolithic coupling scheme.
action: We mentioned it in the text.

Line 327: although this is stated at the very end of the paper it should be discussed already here: when using a 2D model its extension in the 3rd direction is 1 m. Therefore the volume considered for the heat source is not realistic. The real occurring temperatures are certainly lower. This should be made very clear. Generally this approach is quite questionable. It would have been better to derive temperatures based on a 3D model occurring within the repository and use these temperatures as time dependent BC instead the heat source. BTW – the temperature given violates the maximum temperature of 100 °C allowed by the StandAG – however BGE increased this value recently to 150 °C.

For a full 3D simulation, temperatures would be lower due to the additional degrees of freedom and thermal dissipation pathways. Nevertheless the overall qualitative behavior observed in the 2D model would remain the same. The overestimation of temperature is conservative measure, which is not uncommon in preliminary safety assessments for repositories.
action: We explain already at this point in the study the problem with the 2D approach, i.e. the overestimation of the temperature.

Line 336: '??'

Thanks for pointing this out.
action: We fixed the figure reference.

Line 340: this uplift is a consequence of the values for the thermal expansion not discussed at all and not referenced in the final table. A little bit more of information would be good.

This information is certainly missing here and should be added. The thermal expansivity is certainly in the final table, but we can reference to it.
action: We explained the reason for the uplift and referenced the thermal expansivity in final table.

Line 475: this is speculative – suggest deletion.

Agreed.
action: Deleted.

Line 487 – 488: speculative – suggest deletion.

Agreed.
action: Deleted.

Line 491: why is it advisable to use a plastic material law for the overburden rocks? Why is the elastic approach not valid? In my opinion elasticity is for these kind of rocks an okay presumption.

Elasto-plasticity might be advisable only if the near surface processes are of interest. May also depend on the geology. E.g. over a salt dome there may be a loosening zone, which is not accurately depicted by an elastic model.
action: None.

Line 555: in http://www.sciencedirect.com/science/article/ pii/S1876610215016422 and https://www.sciencedirect.com/science/article/pii/S0309170817307510 approaches are shown to model the movement of the freezing (thawing) front using an adaptive mesh refinement. Such an approach should at least be mentioned as it helps a lot by mitigating the mentioned numerical problems.

Good suggestion!
action: Added this approach as a possible solution.

Line 570: ‘the following figures’ – which?

On the following page, the text got removed from figure during optimization of manuscript layout.
action: Reference the figures by numbers.

Table 5: why is the Biot coefficient for Buntsandstein 0.5 while it is 0.6 for the remaining rocks. To my knowledge it is very challenging to obtain valid Biot coefficients. Literature typically refers to 0.6. For conversativity also 1 might be suitable.

Indeed its determination is challenging. We adopted the values given in the Resus reports and decided not to deviate from them for single rock types for this study.
action: Added a note to the material property table, specifying where the values come from.

Lack of phase change: it is indeed a short-coming of this study that the significant decrease of hydraulic conductivity due to to phase change is not considered. Actually it wouldn’t have been too difficult to set K to a value say 1E-6 times smaller in case T < 0 °C.

This is already discussed in Appendix B. In the current setting this added a lot of non-linearity to the model due to freezing-dependent permeability values and did not add much insights for the deeper layers. To avoid having to use further counter measures like e.g. adaptive mesh refinement which went beyond the scope of this study, we decided not to use this feature.
action: We added further information and references to the corresponding section in the appendix.

Model philosophy: performance vs. accuracy: this is mentioned several times in the paper for justification of model simplifications – i.e. they are necessary for performance reasons. However, it remains somewhat unclear which decrease of performance is meant. When is performance decrease relevant enough for justifying relevant model simplifications?

Thank you for raising this point, which is one of the key questions in modeling and also associated with practical constraints in research projects. Our main objective here was to establish workflows for this type of simulations that allow reproducible and automated simulations. As a consequence, several model choices were motivated not just by saving computational time but also by having a meaningful, yet manageable computational representation that could serve as the prototype for such a workflow. In actual barrier integrity analyses some of the choices would certainly be made differently.
action: None.

Finally: have there been any mesh convergence studies? Quite often sensitivity studies are part of such model studies (I don’t say that they are always relevant) – is there a reason this is missing here?

There are and they can all be found in the final report of the research project. In fact, one of the main advantages of the automated workflow is that mesh convergence studies can be performed efficiently. We currently have a companion paper under review, that contains some of those results.
action: We added a section regarding the convergence behavior to the appendix.

Review Round 2

Reviewer 1 (anonymous)

All reviewer comments have been carefully regarded by the authors. There are only some new layout errors in the pdf, where some lines are too long, but that should be easy to correct for the final version.

Reviewer 2 (Ayman Abed)

The authors have sufficiently addressed my comments one by one, and I am satisfied with their responses. I therefore recommend that the manuscript be published in OpenGeomechanics in its current form.

Reviewer 3 (anonymous)

I checked the revised submission.

I have no further comments.

Author Response

Great, please publish it.