Rebuttal

Anonymous Referee #1

Note: Reviewer's comments are grey, responses in black.

1) Permeability model of the host rock

I am not convinced that the described porosity-dependent permeability model for the host rock is reasonable to represent a low-permeability shale. Shales are commonly described as a low-permeability rock; e.g., Goral et al., 2020 (doi.org/10.1038/s41598-019-56885-y) state a maximum permeability typically less than 1000 nD (~9.8E-19 m2), which would not allow for significant advection (e.g., Ingebritsen et al., 2010; doi.org/10.1029/2009RG000287).

If there is no field evidence for these highly permeable shales in the Neuquén Basin,the presented models are not appropriate to interpret the igneous petroleum system and hydrocarbon transport in the Río Grande Valley. In that case, I would like to request the authors to either (1) refer to the host rock as a more permeable rock type (e.g., sandstone) that matches a permeability of ~1E-16 – 1E-14 m2, or (2) to test/proof if simulations with host rock permeabilities of < ~1E-18 m2 would give similar results as presented and discussed in this contribution.

In the prior case, the changed host rock type should be considered in the discussion. E.g., What are the effects on organic matter transformation to methane compared to shale? Due to the change in host rock, the presented flow simulations would further not represent the field locality such that an interpretation of the implications for igneous petroleum systems in the Río Grande Valley may not be feasible.

We agree with the reviewer and accept this criticism. Therefore, we provide two new runs (with impermeable and permeable sill) with a significantly lower host rock permeability. The values are at ~10^{-18} m^2 at sill emplacement depth. We add this to our simulation results (section 3.4.2) and discussion (section 4.2), which we revised overall to incorporate all comments. Thus, our contribution now provides a comparison between high and low permeability host rocks.

The overall results and conclusions remain largely similar, with some added complexity for the low-permeability case. This is because extensive hydrofracturing compensates much of the reduced permeability and thereby facilitates flow. For even lower permeabilities, this compensation effect should be even stronger. As the shales in the study area show extensive networks of (hydrothermal) veins, we think that the new runs show quite plausible behaviour. The hydrofracturing process itself adds a new layer of complexity, which necessitates a detailed description. Please refer to the overhauled result and discussion sections.

The new results allow us to maintain most of our interpretation for low-permeability systems such as the Neuquén case, while also providing insight into systems with higher or intermediate permeability (results from original manuscript).

We did not change the organic matter content in the host rock in order to limit the number of parameters that are changed between the scenarios. However, we do see a small effect on overall generated methane for the two host rocks, mainly due to stronger heat advection in the high-permeability host.

While reading the section on host rock permeability, I was wondering why no brittle-ductile transition (BDT) was implemented for the host rock? Other studies on hydrothermal fluid flow suggest a BDT starting at temperatures of 360 ºC (e.g., Hayba and Ingebritsen, 1997; doi.org/10.1029/97JB00552). Would a BDT in the host rock decrease the permeability within the high-temperature aureole and thus affect fluid flow pathways?

We thank the reviewer for this comment and the valuable resource, especially as host permeability is also discussed. In fact, a brittle-ductile transition for the host rock ranging from 500-750°C is implemented in the model but was not specifically mentioned in section 3. Note that except for the three modifications (only tensile failure mode, hydrofracturing affecting permeability and porosity, cooling joint formation) our model is identical to the one presented by Galerne and Hasenclever (2019). We have clarified this in section 3.

Due to the thin sill and relatively low emplacement temperature, the effects are very limited in time and space, only 5-10 m of the aureole reach >500°C and only for a few years. Maximum temperature at the contact is ca. 670°C, such that full ductile permeability reduction is never reached. Of course, if the BDT were to start at lower temperature, as suggested in paper mentioned by the reviewer, the impact of this could be more pronounced and could be tested. We may add that in the study area, the evidence of ductile behavior in the high-temperature aureole is limited to the first few decimeters of the contact (e.g., Rabbel et al. 2021).

2) Permeability model of the intrusion

Please provide more information on how the dynamic permeability within the intrusion is calculated. At the moment it is a bit unclear to me.

For your setup, I understand that the intrusion is impermeable (1E-20 m2) at T>=1100ºC. Using the described linearised, temperature-dependent definition of the melt fraction, a crystallinity of 50% is reached at T=1000 ºC, which is the BDT and defines the onset of fracturing due to cooling. The next step is not clear to me. Does the permeability linearly increase during cooling until T=900 ºC is reached where the intrusion reaches the maximum permeability (1E-15 m2)? Is that correct? If so, the authors could refer to Iyer et al. (2013) who used a similar linear permeability approximation in one of their models.

Yes, this is how it is implemented in our model: We parameterize the cooling joint formation as a linear transition between 1000 ºC (zero porosity, zero permeability) and 900 ºC (8% porosity, 1E-15 m^2). There is, however, a significant difference between our parameterization of cooling joint formation and the one by Iyer et al. (2013), which we now reference: We not only increase permeability but also porosity, which is more realistic and affects pore pressure evolution as well as methane transport.

We added a sketch to illustrate the simple linear permeability model employed (Figure 5c). We also revised the description of the model (section 3.2 "Adjustments for this study").

Including the permeabilities of the intrusion for the threshold temperatures (T=1000 ºC, T=900 ºC) within the manuscript could also help to clarify the permeability model.

See answer above, we added a graph for clarification (Figure 5c).

I would further like to invite the authors to justify and discuss the permeability values chosen for the fractured intrusion (1E-15 m2). Measured permeabilities of fractured intrusions within the Neuquén Basin (Spacapan et al., 2020) indicate permeabilities of ~5E-18 to 5E-15 m2, with the majority of the samples being <5E-16 m2. In their models, the authors use a permeability of 1E-15 m2 for a fully solidified and fractured intrusion.

Although this is only slightly above the maximum permeability reported by Spacapan et al. (2020), I would like to invite the authors to discuss potential effects of lower permeabilities as observed within intrusions in the Neuquén Basin on fluid flow and hydrocarbon transport. Would there be a fluid flow Phase 2 ("flushing") also for permeabilities of <=1E-16 m2 ?

This is a valid comment, the justification of the permeability choice is not clear enough and has been updated in the revised manuscript (section 3.3, third paragraph). We chose Spacapan as the local reference, because it is the only real-world data we have. Spacapan's maximum value as stated by the reviewer is 5E-15, so our 1E-15 are in fact a bit below (not above) Spacapan's (2020) maximum values. We chose 1E-15 as the permeability to be at the upper end of Spacapan's values to make the sill a permeable medium comparable to the local producing sills. However, this likely still comes short of the real values (which we simply do not know), but they are probably higher still, because the values derived by Spacapan are core measurements. Macroscopic cooling joints or hydrofractures will provide much more efficient flow paths – but explicit fracture flow is not possible in the already complex hydrothermal model. Thus, we believe that 1E-15 is a sufficiently high value to term the sills "permeable".

The manuscript explores exactly this difference by comparing the permeable sills to non/very low-permeable sills, where we set permeability to 1E-20, so essentially 0, as a lower boundary. As shown in by the reference runs (Figure 6 and 7), fluid overpressure cannot be released through the impermeable sills upwards in such a case, and the fluids would need to take the route

via the sill tip. This is the “standard” assumption in most sill modelling work and therefore the reference.

As discussed in previous studies, permeability is a key controlling parameter within hydrothermal systems; e.g., the limiting permeability that allows for significant heat advection is 1E-16 m2 (e.g., Ingebritsen et al., 2010). Therefore, it is critical to carefully decide on (and justify) the permeabilities used for both the host rock and the solidified intrusion as they will control the dynamics of the whole hydrothermal system including maturation and methane transport.

The value of 1E-16m^2 is the limit below which heat advection vanishes and heat conduction dominates for bottom-heated magmatic hydrothermal systems. In such systems hydrothermal circulation is solely driven by the buoyancy differences between cold recharge flow and hot hydrothermal upflow. In the case of sill emplacement in sedimentary rocks, there are additional forces driving fluid flow: clay mineral dehydration and organic matter transformation release fluid mass into the pore space, leading to much higher pore pressures compared to a buoyancy driven hydrothermal convection system. As a result of these strong pressure gradients, significant fluid flow also occurs at permeabilities lower than 1E-16 m^2. If hydrofracturing is considered, the fluid flow is further enhanced even in rocks with permeabilities as low as 1E-18 m^2.

3) Model description

The authors refer to Galerne and Hasenclever (2019) when describing the model. However, a more detailed description of the model including the governing equations would be beneficial, given that this is the focus of the manuscript. This section could also be provided as appendix.

We understand the desire to present the model in more detail. Yet, since we use the identical model with the same parameters – except for the changes that we describe in section 3.2 – providing the entire model description in our study again would mean to copy & paste several pages of (Galerne and Hasenclever, 2019) into an appendix. We believe this is not necessary, because the study by Galerne and Hasenclever (2019) is a free-access publication in a well-known international journal. We have extended the description of the modifications made for this study.

In addition, simplifications and assumptions of the model setup could be introduced and justified here (Section 3.1). The model considers a single-phase flow of a compressible fluid following Darcy’s law (L 251-252). From Galerne and Hasenclever (2019), I learned: “Throughout the calculations, pore pressures are above the critical point of pure water so that the fluid remains in a single-phase state. Our single-phase hydrothermal model requires this assumption, because in

the system H2O–NaCl–CO2–CH4 phase transitions would be possible even at higher pressures.”. This assumption should be included and explained in the presented manuscript, and potential effects on the modelling results should be considered and discussed later in the manuscript. Given the shallow emplacement depth of 1-3 km, pore fluid boiling is plausible. Would this phase transition change fluid flow patterns and the transport and accumulation of the hydrocarbons?

We now only consider deeper sills at 3 km depth because they are more representative for our case study. Whether phase transitions could occur near the sill depends on the salinity of the fluid. Pure water would be above its critical point hence would remain in the super-critical single-phase state. Saltwater, on the other hand, could potentially undergo phase transitions. However, we find strong overpressures developing in the contact aureole (up to ~90 MPa, where cold hydrostatic pressure is 30 MPa), so that even salt water may remain in the high-P, high-T single-phase region. Assuming a typical seawater salinity of 3.2 wt.% NaCl, the phase diagram below (calculated using the equation-of-state by Driesner & Heinrich, 2007) shows that boiling at 30 MPa starts at ~410 ºC, while at 90 MPa it starts at ~640 ºC. But all this is speculative, because salinities will change once phase transition and phase separation occur, and a multi-phase hydrothermal model would be required to further elaborate on this question, which is beyond the scope of our study.

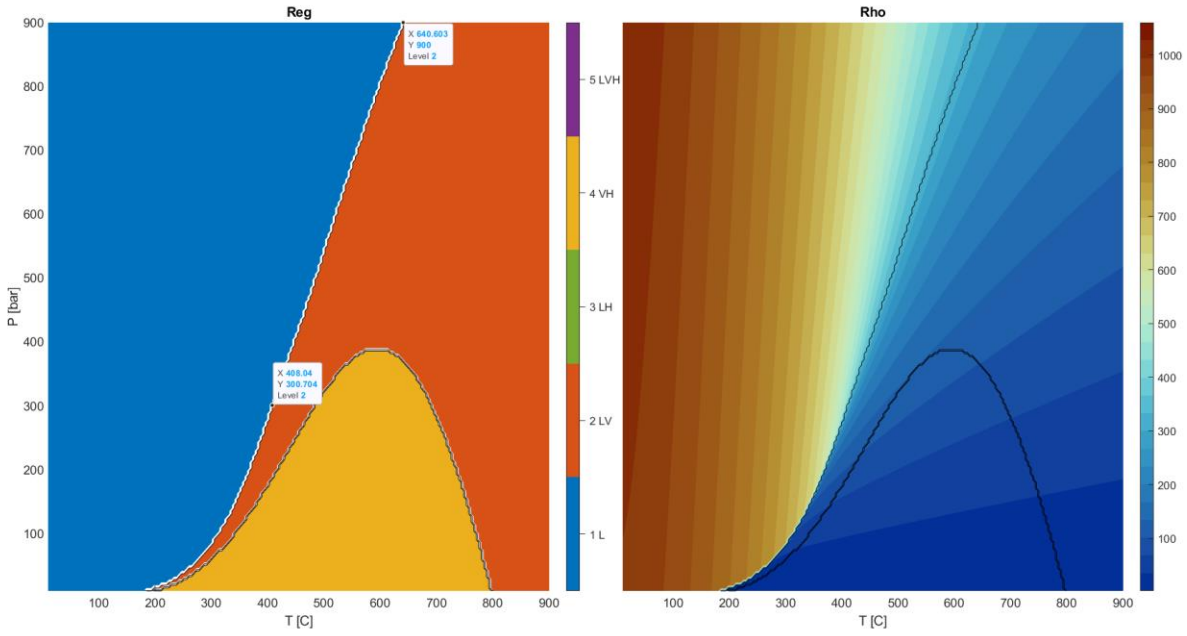

Figure 1: Phase regions (left) and bulk density (right) of seawater (H_2O with 3.2 wt.% NaCl) based on the equation-of-state by Driesner & Heinrich, (2007). Phase regions are: L – single-phase, LV – liquid+vapor coexistence, LH – liquid+halite coexistence, VH – vapor+halite coexistence, LVH – liquid+vapor+halite coexistence. The phase boundary L/LV is pressure dependent and would change by several hundred degrees during the pore pressure build-up after sill emplacement.

Buoyancy effects caused by methane in the fluid are not considered in the models (L 262-264). Is this because the effects are too minor to significantly affect fluid flow or would buoyancy change the modelling results?

We have not tested whether additional buoyancy effects of methane may change our modelling results. Although the lack of buoyancy effects certainly represents a model limitation, we point out that Iyer et al. (2013) found no significant changes in methane discharge in their model comparison with either weak or strong CH_4-related density reductions. A reliable equation-of-state for H2O–NaCl–CO2–CH4 is missing and prescribing an ad hoc density change depending on CH_4 concentrations bears the danger of oversimplifying the actual fluid density evolution. We therefore decided to not implement supposed density changes but to use the equation-of-state of pure water (cf. Galerne & Hasenclever, 2019)

The exact domain size of the models is not given and should be included in the model description. It would also be important to explain/show how far away from the sill tip the no flow boundary is located.

We improved figure 5 and provide the information in the text.

Is the element size of 0.5 m consistent throughout the whole domain or only in a refined area within and around the intrusion?

We now show the mesh resolution in figure 5.

4) Results and Figures

The figures are of good quality and visualise the results described in the manuscript. However, not all data discussed in the text are presented in the figures (Fig. 6, 7, 8, 9). Fluid pressure and the pore pressure distribution are both used to explain changes within the distinct fluid flow phases (i.e., “flushing” and “post-flushing”) and are also used throughout the discussion to explain fluid flow and methane transport. Therefore, these parameters are essential and should be presented in the manuscript. Although velocity vectors are presented in Figure 8a, it would be great to also include these vectors for all models shown in Figures 6, 7, and 9.

We thank the reviewer for this comment, the pore fluid pressure (distribution) is certainly at the heart of the process interpretation. We changed the displayed data in the Figures 6,7,8,9 (half-sill view for low/high-permeability hosts with impermeable/permeable sills). The updated panels are as follows:

1. Row: Temperature and maturity
2. Pore pressure and flow vectors
3. Permeability and transient fracture porosity (to indicate distribution and intensity of hydrofracturing)

4. Methane distribution as Fluid fraction with flow vectors

The new close-up figure 10 displays pore fluid pressure and permeability/fracture porosity in the same style. We also adjusted the colorbars according to the recommendations made by the reviewer in the annotated pdf, i.e., we use fewer color levels and provide contour labels where we deemed it useful.

The updated figures are also referred to in the updated results (sections 3.4.1, 3.4.2) and discussion (section 4).

I would also like to invite the authors to provide videos of a representative simulation of both a permeable and impermeable sill as supplemental material. These videos could visualise fluid pressure, temperature, CH4 concentration, and velocity vectors, which would allow the reader to see how the fluid flow evolves over time and how the described phases of fluid flow form.

This is a good suggestion; several videos are provided as supplements and are referenced in the text. This gives the reader a much better idea of the dynamics of the phases over time and space.

5) Discussion

This section is a good summary of the distinct fluid flow phases observed in the models, but it misses some explanation on which mechanisms or physical parameters control each phase. For example, it is not clear, which mechanism causes a contact-parallel flow in Phase 1. In Section 4.4, the authors suggest that impermeable sills favour fluid pressure build-up and contact-parallel flow toward the sill tips. This explanation should be extended and data to support this interpretation should be included in the manuscript.

We hope that the added data (see above response) and improved description in the result (section 3.4.1) and discussion sections make the interpretation clearer. We would like to add that pore pressure build-up around sills (particularly those emplaced in organic-rich sedimentary rocks), is a well-documented phenomenon (e.g., Aarnes et al., 2012, Iyer et al. 2013, 2017, Galerne and Hasenclever 2019). In the lower aureole, the fluids cannot escape upwards as long as the sill remains (partly) impermeable. This leads to flow towards the edges of the sill. This contact-parallel flow of fluids from below the sill toward the tips is at the center of the theory for formation of (explosive) hydrothermal vents, so our interpretation of Phase 1 is more a repetition of previous work (e.g., Iyer et al., 2017).

In Phase 2, pore fluid pressure (overpressure and rapid pressure dissipation after the formation of cooling joints) is used to explain the upward-directed fluid flow and hydrothermal “flushing”. As

mentioned above, I would like to request the authors to provide data to support this interpretation.

See replies above. We acknowledge the need for this data to support our interpretation and now provide data on pore fluid pressure in both overview (half-sill view) and close-up figures (6-10).

It is also not clear to me how the change in pore pressure distribution initiates the vortex flow in Phase 3. Again, no data is provided to support this interpretation and the mechanism that initiates the vortex flow should be described and discussed in more detail.

We extended the discussion of the vortex slightly, but want to avoid too much focus on this phenomenon, as it is not clear how pronounced it would be in a more realistic scenario, e.g., with lithology variations. In section 4.2, we therefore also renamed the third phase as "stabilization and fading hydrothermal flow" to put less emphasis on the vortex feature.

The focus of this work remains to highlight the possibility for, and potential importance of, permeable pathways through intrusions shortly after solidification. Once our model includes further complexities (e.g., multiphase flow, mineral precipitation, BDT, or realistic geology), it would be interesting to investigate if this feature persists

Discussion - Impact of permeable sills on hydrothermal flow

As mentioned in comments 1 and 2, permeability is a key controlling parameter that affects hydrothermal systems. This section should therefore discuss how different permeabilities would affect the described flow phases. Do the individual flow phases also form for low-permeability host rocks (k <1E-16 m2) and sill permeabilities as described by Spacapan et al. (2020)?

Again, we thank the reviewer for this comment, and realized that another simulation with lower permeability was necessary to understand the implications of permeable sills on hydrothermal flow. Figures 8 and 10 show the flow patterns for a low-permeability host with a permeable intrusion, and the flow phases are described in section 3.4.2 and discussed in section 4.2.
For a permeable sill in a low-permeable host rock (<< 1E-16, see Figure 5b, 8, 10), flow phases 1 and 2 are quite similar to the higher-permeable host rock, while more complex due to hydrofracturing. A key observation is that there is still fluid flow in a lower permeability host, because hydraulic fracturing is more pronounced and elevates permeability (and porosity). In our model, the permeability increase has a limit to 2 orders of magnitude above reference permeability, somewhat limiting the flow overall. Nevertheless, this shows that hydrofracturing around sills can generate create sufficient permeability even in low permeable rocks like shale. In fact, the outcrops of sills emplaced in shale which we visited in Neuquén show networks of hydrothermal veins in the shale (possibly hydrothermal, compare Spacapan et al., 2019, and

Rabbel et al., 2021). One might speculate that at least part of these veins are remnants of this process.

For much lower sill permeabilities refer to the comments above – we present a case for an impermeable sill in Figure 6. Here, we do not see the same flow phases, and the main difference at lower host rock permeability is that hydraulic fracturing is sustained for longer, which in turns increases permeability. Iyer et al (2017) investigated such a case for a large-scale sill complex offshore Norway.

Discussion - Implications for igneous petroleum systems in the Río Grande Valley

Based on the permeabilities used by the authors, I am not convinced that it is feasible to discuss implications for the described field location (please see comments 1 and 2).

Again, this is a valid point and the authors are grateful to take this opportunity to provide new simulations to facilitate the interpretation with respect to Rio Grande Valley. In our view, the new simulations provide scenarios that are suitable to discuss implications for the sills of Rio Grande Valley. Overall, we reduced the discussion for Rio Grande Valley (section 4.4) to the impact of hydrocarbon "flushing", as we believe that this is the main point worth discussing in this context.

References that are not in the manuscript:

Driesner, T., Heinrich, C.A., 2007. The system H2O–NaCl. Part I: Correlation formulae for phase relations in temperature–pressure–composition space from 0 to 1000°C, 0 to 5000bar, and 0 to 1 XNaCl. Geochim. Cosmochim. Acta 71, 4880–4901. doi:10.1016/j.gca.2006.01.033