Response to reviewer comments on ‘Numerical modeling of CO_2 fracturing by the phase field approach’

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We thank the reviewers for their constructive comments to render the manuscript with higher quality. Below we first respond to each of the comments with the original comments italicized, then summarize the major changes of the manuscript. However, since this is an extensive revision, we will not provide a detailed list of changes since that would mean an extensive repetition of the text. Here we only bring to the editor’s and reviewers’ attention that we have merged the former Appendix A into the first three subsections of Section 4 to make the latter following an order from simple examples to complicated ones. Also note that all other changes in the manuscript are marked in blue.

Comments from Reviewer #1

In overall, the manuscript is well written. I would recommend this manuscript for further consideration if the authors make the following revisions:

The nomenclature should be consistent with SPE nomenclature, for example v should be used for velocity instead of q, l should be used for length instead of σ.

We appreciate the reviewer’s positive comment. Following the SPE nomenclature, now we have substituted $\mathbf{v}$ for $\mathbf{q}$. Following the convention of the phase field for fracture community, we reserve ℓ for the regularization length scale. Note that σ is nowhere used for length but for the *in situ* stress.

When CO_2 flow in the fracture and in rock, there are more than one phase because formation fluids also flow, hence the formulation should be for at least two phase.

It is true that including more phases would lead to a more realistic model. Moreover, our formulation for CO_2 as a compressible fluid is applicable to more than one phase with minimal changes. This being said, however, there are cases

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in which one phase is sufficient, and which is the scope of the proposed method in its current form, because the more complex the model, the more difficult to verify and validate. So at this stage, we confine ourselves to the simpler case of one phase to carefully verify the model, and generalization to more phases can be a future step. More precisely, it will be assumed that CO_2 is in its supercritical state, and as the shale is a deep reservoir, the size of the fluid lag is negligible. In the revision we added the limitation of the proposed method at the end of Section 2.

Please use a consistent color set for all figures, scale in some figures changes white to black while others change from blue to white.

We have edited Figure 1. The color bars are now from blue to red everywhere. It is also worth mentioning that in the current Section 4.1 the initial cracks are explicitly imposed, so that in the deformed configuration in Figure 4 they appear as lines in the color of the background (in the normal case white). See the caption of Figure 4.

Please include a short paragraph to show how d and α_k (Eq. 9) are determined?

The phase field d is the key parameter in the phase field approach. It is obtained by minimizing (3), holding other fields fixed, which leads to the weak form, now numbered (A.1b). The solution procedure is given in Section 3, in which it is elaborated how the phase field d is solved while coupled to $\boldsymbol{u}$ and p. The current Appendix A.1 gives the discretized form for the residual vectors and tangent stiffness matrices for solving d as well as $\boldsymbol{u}$.

The parameter α_k is a parameter to input. We have expanded the paragraph surrounding Equation (9) to explain this point.

Please use more close to reservoir condition for input data. The tensile strength in Tab. 1 is very high for the rock with that Young's modulus. The initial pressure is rather too low.

Since we aimed to verify our results with Wang *et al.* [1], the selected input data are in accordance with this reference. Also, all mechanical input data are approximately within the range proposed for the shale in a few references. See, e.g., Table 1 for a comparison between our input data with the suggested mechanical properties for the shale by Eseme *et al.* [2], in which the authors reviewed literature on the mechanical properties of oil shales. Also, the initial pressure is in accordance with [1].

Table 1: Mechanical properties of rich shale from the Western US.

Property	Symbol	Unit	Values from [2]	Our values
Young's modulus	E	GPa	4.5 ± 0.5	6
Poisson's ratio	ν	–	0.35	0.34
Tensile strength	σ_t	MPa	9.5 ± 1.5	11

Please include all necessary inputs for the simulation to allow other people to duplicate the job if needed. There is no data related to in-situ stresses. Although, they are not in the equation but they are the boundary condition.

We found we missed in one place the values of *in situ* stresses, which we have added on p. 22, l. 341. We believe now all other input data and the algorithm are sufficient for reproducing the results.

More numerical simulation or case studies may be needed and a comparison with other models may be useful to show the innovation of this model.

What makes the phase field an attractive approach can be attributed to its convenience in simulating complex fracture processes, including crack initiation, propagation, branching and merging. Compared to discrete crack descriptions, the phase field approaches avoid tracking the complicated crack geometry; instead, the crack evolution is a natural outcome of the numerical solution to a constrained optimization problem. Thus, it significantly decreases the implementation difficulty, especially when dealing with 3D problems. To illustrate this major advantage, in this version, we added two more application examples to the manuscript; (1) increasing pressure leading to joining cracks, as Section 4.4, and (2) interaction between CO_2-driven fractures and inclined natural fractures, as Section 4.6. Both examples result in complicated crack topologies. At the end of Section 2, we also added a paragraph to discuss the innovation of the current model.

We need more section to discuss the advantage of the model compared to other approaches.

We added one paragraph to the end of Section 2 to discuss the advantages as well as limitations of the current approach.

Comments from Reviewer #2

This paper presents a very novel approach to model the CO_2 fracturing process. I think this topic is very new and definitely worth digging into. The authors have presented enough details about the fundamentals of the solution, and overall I think this paper is very well laid out. I have following minor suggestions for further improvement:

1. One main concern is that this paper seems too mathematical.

We appreciate the reviewer's positive comments. Since the objective of this paper is to propose a *numerical* model for CO_2 fracturing, we had to provide necessary formulas in a way that readers can reproduce our results.

The layout of the manuscript could benefit from more description about the application of the methodology.

We added two more application examples to the manuscript; (1) increasing pressure leading to joining cracks, as Section 4.4, and (2) interaction between CO_2-driven fractures and inclined natural fractures, as Section 4.6.

2. The validation is not very clear to me. The author presented three verifications, but are they trying to prove the validity of the proposed method? Honestly I didn't recognize the method that was used for validation. Is it a well-established analytic solution, or results from well-established simulation? I would strongly recommend re-write the validation part.

Yes, we were trying to prove the validity of the proposed method in the former Appendix A, which is now Sections 4.1 – 4.3. In these three sets of examples, we compare our method against exact or otherwise well-established solutions for verification. See Table 2 for a summary of the requested information by the reviewer. In addition, we made some minor edits to these sections to clarify these issues.

Table 2: Summary of the verification examples.

Section in the revised manuscript	Reference solution	Type
4.1	Miehe *et al.* [3]	Numerical
4.2	Detourney and Cheng [4]	Analytical
4.3	Sneddon and Lowengrub [5]	Analytical

3. What is the limitation of the current method?

The limitation is the rather simple model for the gas flow and permeability in shale media. We added a summary of the limitations as well as the advantages at the end of Section 2.

It is not very clear to me that whether this method is application to traditional water based fracking or not.

The phase field approach has already been applied to water based fracking by multiple authors, see e.g., [6, 7, 8, 9, 10, 11, 12, 13].

And if so, what is the advantage of the current approach?

The advantage of the current approach is the generalization to *CO_2 fracturing*. In the paper at hand, we propose a phase field model to consider CO_2 as a compressible fracturing fluid under the isothermal condition, as the first step towards such modeling. More precisely, the CO_2 density varies significantly with pressure, which is captured by the Span-Wagner equation of state [14]. The computed values show good agreement with analytical solutions and experimental results.

Comments from Reviewer #3

The paper tries to use phase field method to model CO_2 fracturing. Some assumptions used in governing equations are not supported with the theory of poroelasticity. Hydraulic fracturing or CO_2 fracturing involves strongly coupled processes. But the authors verify their model through non-coupled examples.

The coupled behaviors about pressure and aperture evolutions are not demonstrated. This makes the correctness of the model in doubt. I recommend resubmission of the paper after the model is correctly verified through asymptotic analytical solutions for hydraulic fracturing. Without correctly verifying the coupled model, I cannot recommend the acceptance of it.

Regarding verification with asymptotic analytical solutions for hydraulic fracturing: The phase field approach has already been applied to hydraulic fracturing by multiple authors since 2012, see e.g., [6, 7, 8, 9, 10, 11, 12, 13]. Among these references, Wilson and Landis [15] and Chukwudozie [16] have already verified the phase field hydraulic fracture models with asymptotic solutions by Detournay and Garagash [17] and Hu and Garagash [18]. They verified the phase field model for both toughness-dominated and viscosity-dominated regimes, and found good agreement for pressure, aperture, and fracture length. At the beginning of Section 4, we now remind the readers of such existing verification results. As the phase field part of our method is based on the literature, and the main innovation is to model CO_2 fracturing by treating CO_2 as a compressible fluid, we did not plan to repeat such verifications for hydraulic fracturing.

The followings are a few comments:

1. The authors used a phase field depended permeability in their study. The permeability should be determined by the opening or close of fractures. Why could a damage variable be used to determine permeability? The phase field value is distributed over a range, however, a fracture creates jump in pressure and displacement. Why could a continuous variable be use to represent discontinuous behaviors, especially for permeability?

In smeared crack approaches such as the phase field method, the discontinuity is distributed over a finite width so that the sharp description of the crack is replaced by a diffusive description. This is precisely the key point of the variational theory of fracture, more commonly called the phase field approach, and its correctness was shown with the language of Γ-convergence, see, for example, Chambolle [19].

In this work, we have used the same idea for the permeability as well. See similar works [20, 21] with a damage model. In this regard, we have expanded the paragraph on p. 7 surrounding Equation (9) for more explanation.

2. Eq. 10 is not correct; which casts doubt on the whole sequentially coupled process. The treatment of porosity in Eq. 10 conflicts with the theory of poroelasticity. Change of porosity is not equal to the change of volumetric strain, not even in an approximate manner.

In [22], Verruijt proved that $\partial_t \varepsilon_v = (1-\phi)\partial_t \phi$, assuming the grains are incompressible. On the other hand, Terzaghi [23] and Sheng *et al.* [24] suggested $\partial_t \varepsilon_v = \partial_t \phi$. In any case, as the porosity is relatively small ($\phi = 0.01$) we can still approximate the change of pore volume to that of the volumetric strain with minimal error. It is also worth mentioning that according to Wang *et al.* [1], the effect of the whole term $\rho \partial_t \phi$ is small compared with other terms.

3. Could the authors give the spatial and temporal discretization in appendix? Since the weak form is given already, spatial discretization is only one step away. I doubt the spatial discretization for a poroelastic medium could be derived from Eq. B1b or Eq. B2b. Though it is possible that the poroelastic model is ready for use in FEniCS package, the authors are suggested to provide the completely discretized formulations for the benefit of readers.

Following the reviewer's comment, now we have added the spatial and temporal discretizations to the current Appendix A. It is true that in our implementation, FEniCS itself computes this step.

4. Fully coupled examples are needed to verify the model. Correctly verifying a tensile test and the pressurization of a fracture do not indicate the model can correctly simulate hydraulic fracturing or CO_2 fracturing. The verification about pressurizing a bore hole is not a good example to show poroelastic responses. Actually, no typical poroelastic responses are shown in the example. Mandel's problem is suggested.

We appreciate the reviewer's suggestion. However, Mandel's problem is based on the assumption that the fluid is incompressible, while our main contribution is to model $\mathrm{CO_2}$ as a compressible flow. Moreover, both being models with incompressible fluids, Mandel's problem would somehow repeat the second verification example (now Section 4.2) where the porous flow is coupled with the porous medium's displacement. Based on these reasons, we would prefer not to carry out Mandel's problem for this manuscript.

5. Please briefly explain the AT1 and AT2 model.

We now explained more about the AT1 and AT2 models on p. 5, under Equation (2).

6. line 1-2 Page 1 Are you sure shale or mudstone is the most common sedimentary rock?

We removed this phrase from the text.

Comments from Reviewer #4

The authors have proposed a model for CO_2 flow and fracturing in shale media. The manuscript has a good order, but needs revision to satisfy publication quality.

Gas flow in shale is one of the most challenging topics and has been widely investigated. The authors have used a relatively simple model for calculation of gas flow and permeability in shale media. A good model will capture important phenomena like Knudsen Diffusion and adsorption effect in shale rock media. Please modify this part of your model by providing a more holistic and detailed explanation. Please refer to series of papers by Javadpour et al. Also see: Seyyed A. Hosseini et al. "Novel Analytical Core-Sample Analysis Indicates Higher Gas Content in Shale-Gas Reservoirs" SPE Journal 2015.

We appreciate the reviewer's positive comments. Regarding phenomena like Knudsen diffusion and adsorption effect, we must recognize that each model has its scale of applicability. The proposed model is applicable to the continuum scale, aiming at simulating complex fracture processes, including fracture initiation, propagation and merging. As this work represents the first of its kind, a relatively simple model is used for the calculation of gas flow and permeability in shale media. For example, we simply used Darcy's law in a viscous flow regime (common in conventional reservoirs), as our continuum approach cannot afford explicitly capturing microscale phenomena like Knudsen diffusion. However there is potential to adopt more sophisticated phenomena like slip flow regime in future works in a multiscale simulation framework. Now we commented in Section 2.2 the works mentioned by the reviewer and admitted to our readers on p. 7, l. 145–150 of the simplicity of the model we used for the flow transport.

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