**Authors’ Reply to Editor of**

**“Assimilation of Geophysics Derived Spatial Data for Model Calibration in Geologic CO2 Sequestration”**

**submitted to SPE Journal**

**SJ-0823-0080**

Dear Executive Editor Silviu Livescu,

We have carefully addressed all the comments from Associate Editor and three technical reviewers. Note that the title has been changed from “Spatial Data Assimilation in Geologic CO2 Sequestration” to “Assimilation of Geophysics Derived Spatial Data for Model Calibration in Geologic CO2 Sequestration” based on a suggestion from the second technical reviewer. We are looking forward to seeing our paper published in SPE Journal.

Sincerely,

*Bailian Chen, Corresponding author*

Earth and Environmental Sciences Division

Los Alamos National Laboratory, USA

**Reply to Associate Editor:**  
  
Two reviewers: TE#2 recommends major changes, while TE #1 still recommends minor revisions. TE#2 has thoroughly reviewed the whole paper and provided very comprehensive review comments. As TE#2 indicated, the framework is pre-existing, and both the method and the problem is known. Thus, the novelty or the distinct contributions of the paper has been largely compromised. One remedies here is to enhance the connection of the findings to some practical questions in uncertainty quantification for geo-sequestration (As TE#2 suggested). Similar concerns were also raised by TE#1 who recommended more defined metrics to evaluate posterior evaluations and enhanced sensitivity study of CO2 error perturbation. TE #2 has also gave many good feedbacks about improving the title, literature, methodology description,  clarity of some points, figures and captions. I concur with these comments and particularly the comment on missing description of the methodology. As TE#2 indicated, although the methods are well established in the literature, but not every readers is a data assimilation expert. Authors should think about a better way to present this section to enhance the general readership of the paper.

* Response: Thanks for emphasizing the major points from the technical reviewers. In the revision, we have addressed all the major comments you mentioned.

**Reply to Technical Editor 1**  
  
The author's response to my previous comments remains insufficient in two key areas.

Firstly, there is a need for a more comprehensive set of metrics to evaluate the posterior evaluations. Secondly, the sensitivity study of CO2 error perturbation, as it currently stands, lacks engagement and depth, making it less compelling. Additional work is necessary to elevate the manuscript to a level suitable for publication.

* Response: Thanks for your comments. In the manuscript, we have presented the CO2 saturation maps evaluated based on posterior models. In the revision, we also added the average mean squared error of ensemble per assimilation step (as shown in Figure 8). Regarding to the sensitivity study of CO2 error perturbation, the idea is very compelling. Technically, it’s very challenging. We don’t have an approach to perturb the CO2 saturation boundary in a 2D area. Even though we don’t know how to do it, we still appreciate the reviewer’s excellent comment.

Furthermore, as highlighted by other reviewers, it is evident that this work is not the pioneering effort in exploring ensemble-based methods for assimilating spatial measurements. To strengthen the novelty of this work, it is necessary that the author considers tackling more intricate cases, seeks to enhance the performance of the ES-MDA algorithm when assimilating large amount of spatial measurements, or explores other uncharted aspects within this research domain.

* Response: We agreed that the ensemble-based methods for data assimilation is not pioneering effort. However, the application of ensemble-based methods especially the state-of-the-art data assimilation approach ES-MDA for geophysics derived spatial measurements in CO2 sequestration is novel. Given the data scarcity in geologic CO2 sequestration (less number of wells comparing to oil & gas industry), the use of spatial measurements in data assimilation to calibrate reservoir models will be very important. We believe that the observations from this paper can be of benefit to the CCUS community.

**Reply to Technical Editor 2:**  
  
After reviewing the paper by Chen et al., I believe that the paper is can be considered for publication after some revisions. The revisions I am asking for seem minor to me because it would only take looking at the data again and perhaps some replotting and additional discussion, but are major in the sense of importance to me as a reader. I recommend this publication as Publishable-Major.  
  
The paper is of importance to the field, of relevance to the readers of SPE Journal, and the objectives, methods and results are presented in a clear manner, although the paper would benefit from more depth of discussion. I enjoyed reading the paper, organization is straightforward. Not having to present the methods makes this paper an easy read, but I wonder if it is acceptable by SPE to not show methods at all. The paper would benefit from some language editing, but I did not spot too many problems.

* Response: Thanks the reviewer for the positive comments on this manuscript.

Specific comments (in the order they appear in the manuscript, not in the order of importance). Asterisks in front of comments indicate that this comment is very important to me as a reader.  
  
Title  
  
The title needs to be more specific and descriptive of the work, e.g., Assimilation of geophysics derived spatial data for state and parameter estimation in Geologic CO2 sequestration. Or something along those lines, but specific enough to point to the methods/data used.

* Response: We agreed with this suggestion. In the revised manuscript, we have changed the title to “Assimilation of Geophysics Derived Spatial Data for Model Calibration in Geologic CO2 Sequestration”.

Abstract:  
  
\*\*Line 15: the framework has been presented before and was previously developed, so it is not novel anymore and it is not developed in this paper, please adjust language. Assimilating all of CO2 saturation datapoints is no different (from a framework perspective) from assimilating well data. Or if it is, it has not been made clear in the paper. The authors say that they assimilate all of the CO2 spatial data, so methodologically, I don’t see how this is different from the previously presented framework. Please clarify.

* Response: Thank you for your comment. Previously, our framework had been applied to monitoring well data, as opposed to the entire field and spatial forecast for data assimilation. It is correct that methodologically it is not different, but in terms of the application of assimilating observed measurements it is indeed a different work than previously proposed. Especially, our observations shows that geophysics derived spatial measurements can be used for better performance of data assimilation or model calibrations than point monitoring well data. To the best of our knowledge, this is the first paper to unveil this in CO2 sequestration.

Line 19: The authors say that spatial data comparatively carry more information, but this is not a fair comparison, and that comparison is not shown in the paper. More data is not always more information, but in this case these are direct state values explicitly linked with both the state and the parameter being estimated. Of course they would carry more information than a few point well data, that is self-evident. The interesting question is how much more information, and do we really need the entire map of saturations and is the accuracy we get from geophysics high enough to provide high accuracy in estimation. It would be useful to deepen the question a little more than presented in the paper, because now it reads as if an existing method and framework was applied to different data and the expected result was obtained.

* Response: Thank you for this suggestion. It would be very interesting to calculate the value of information or entropy in assimilation spatial data as opposed to point data. However, that is out of the scope of this manuscript, but will be considered for future work.

Introduction:  
  
Page 2 Line 3: NRAP-Open-IAM needs to be at least explained – not everybody knows what it is.

* Response: Thank you for this suggestion. We have added a sentence explaining NRAP-Open-IAM.

\*\*Page 2 Line 29: Using geophysical data for CO2 data assimilation is not new. Using spatial data may be newer, but there are definitely examples in closely adjacent fields (see Kang et al., WRR and references therein, or the work of Jonghyun Lee et al on how to handle large datasets in data assimilation). The question of using maps in data assimilation exists in many areas, not just CO2 sequestration and oil, and the literature review should include these works since the method is the same. In addition, this paragraph would be a good point to explain how spatial data is different from well data. Yes more information, but correlated information. Challenges with using large datasets in the data vector. Error propagation from geophysical inversion. There are several interesting questions that affect the practical applications of this work.

* Response: thank you for the suggestions. We have included several references for spatial data assimilation in adjacent fields in the Introduction section.

Page 2: The methodology of the framework is not presented in this paper, which is fine for me being well versed in the specific area, but I do not know if it will be fine for the average reader of SPE. I defer to the editors. The methods are well established and known in data assimilation, but not every reader is a data assimilation expert.

* Response: Thank you for your suggestion. We have included details about ES-MDA-GEO in the Methodology section.

Page 3 - Line 30: “equivalent permeability distribution” do you mean that the same probability distribution/variogram was used to generate each layer, or that you generated the layers using a 3D variogram with the same PDF across the entire domain? Or that the layers are repeated? Unclear and difficult to check since no graph of the domain is given.

* Response: Thank you for the clarification question. The bottom 10 layers are repetitions of the first layer, such that all 11 layers have an equivalent permeability (spatial) distribution.

Page 4 - Line 35: “we only focus on ..” The ensemble standard deviation shows zero uncertainty at the point of the wells. This makes me wonder if you are conditioning the field on known information at the well, and what information that would be. In that sense, are you using only the CO2 maps, or are you also using well data? Have you tried using only one at a time, and both combined to compare the relative worth of information?

* Response: Thank you for the clarification question. When generating the 101 random realizations of the permeability distribution, we keep the location of the wells constant. At these locations, the value of permeability is known, and therefore the 101 realizations will have the same value, thus zero uncertainty at the point of the wells.

We have included clarification of this in the first paragraph of the “Case Study and Results” section.

Figure 6: it would be useful to show differences spatially to identify where the benefit is most pronounced. Second column is given the name “prior”. Based on the caption, these are the data used, so I am not sure that it is technically the prior. The prior would be the prior distribution assumed for CO2 at the beginning of data assimilation. Which makes me wonder, what was the prior used for CO2 (it is specified for perm). The term “prior” becomes even more tricky if you consider that in the next figure you use the term “prior map” for a different field. Given that prior has a specific meaning in the context of ensemble data assimilation, please use specific words with more descriptive language.

* Response: Thank you for your comment. In this case, the prior maps represent the CO2 distribution from the random realizations in the ensemble without any data assimilation. The “observational” column represents the ground truth measurements, and the “history matched” column is the simulation of the prior/realization after performing spatial data assimilation, or the posterior. Therefore, our priors are not representative of the observational data, but after our data assimilation procedure, the priors are updated to match the ground truth and their forward simulation will match the observational data.

Figures 7 and onward: Captions need to be much more descriptive and standalone as was done in figures 1-6.

* Response: Thank you for your comment. We have expanded the figure captions to be more descriptive.

Page 7 – line 1: “updated reservoir model” while this is semantics, it is good to be specific. It is better to say “the reservoir model with updated permeability field” since only permeability was updated in the reservoir model.

* Response: thank you for your comment. We have changed “updated reservoir model” for “the reservoir model with updated permeability field” to clearly state that the permeability field is being updated and the CO2 distribution is the simulated response of the updated field.

Page 7 line 5: missing word Figure

* Response: thank you for your comment. We apologize for this typo and have included the word Figure in the sentence.

\*\*\*Page 8 line 6-8: Does the error of inverted seismic data work this way? Is the error in a geophysical inversion (seismic--> CO2) Gaussian? In this case, was the random error added and the 1% is the standard deviation of the gaussian error added on top of the saturation maps, or was the error incorporated in the processing of the seismic data? Which makes me also wonder, how did you go from seismic data to CO2 maps?

* Response: This is a great question. We don’t know the type of distribution of geophysical inversion. In our analysis, we assume the error is in Guassian. In our study, the standard deviation of the Gaussian error was added on top of the saturation maps. To go from seismic data to CO2 distribution, one can apply a fluid substitution model such as the Gassmann equations. However, we assume that this is already given to us and we can work directly with the permeability and CO2 saturation distributions.

\*\*\*Figure 9: I do not discern any difference between the three columns, which is concerning. At least a map of the differences needs to be shown. Theoretically, the added noise should translate to more uncertainty. Did the uncertainty maps change? They are not shown. If they did not, there is a mistake in the code. When a DA code does not produce any difference with different input data it can either be theoretically explained, or it is a mistake in the implementation. Please doublecheck and show uncertainty maps too, as well as differences in estimation.

Response: Thanks for your comment. First of all, there is no mistake in the implementation. We are glad to see even the expert reviewer cannot distinguish the difference among different plots, which further implies that for the level of uncertainty associated with seismic data interpretation used in this study, the uncertainty in the updated permeability distribution is not significant. We chose two regions in the four plots noted below to show that all the plots do have difference. However, the differences are small. The observations here show the robustness of the geophysics derived spatial measurements for data assimilation.

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Conclusions  
  
Line 14: The only result that shows reduction of uncertainty in the paper is Figures 5 and 8, and they both show reduction with additional spatial data incorporated. More data will result in some reduction to uncertainty always. What is the argument here? Are the authors trying to see how many geophysical surveys it will take to reach a certain improvement in uncertainty reduction? Did they try with 4 surveys to make the point that 3 was enough? Are the authors trying to say that there is more uncertainty reduction than with well data? It is expected that there is, but is this shown in the paper? And is it even worth to use well data? Do we know what the uncertainty reduction is with only well data and with combined data? How do this different data change the risk uncertainty maps that the authors say is connected to their algorithm?

* Response: thank you for your comments. We have included more details in the Conclusions section to address these questions.

I really wish the authors tried to connect their findings with some practical questions in uncertainty quantification for geologic CO2 sequestration, especially since the method is known, the problem is known and the framework is pre-existing, so the novelty of the paper could be in the contribution for applied projects. The paper begins by saying that this framework is used within the NRAP risk framework, but I don’t risk error propagation mentioned in the conclusions.

* Response: Thank you for your comment. We have included a connection to field applications and large-scale GCS operations, and the usage within NRAP-Open-IAM software.

References: the list of references does not include work that uses the same method in other related fields. Please see previous comments.

* Response: Thank you for your comment. We have included references to other works that use a similar procedure for spatial data assimilation.

Typos:  
Page 2 Line 8: multiple approache\*s\*  
Page 2 Line 18: site\*s\*  
Page 5 – line 5: Figures 4 and 5

* Response: Thanks. The typos were fixed.

**Reply to Technical Editor 3**  
  
This paper deals with data assimilation using saturation maps for CO2 sequestration. The authors used ES-MDA-GEO for history matching to update permeability models. They analyzed the effect of the number of spatial data and the effect of noise level in saturation maps. The overall flow of the paper is well-written, but several key information for the methodology is missing in the current manuscript and additional analysis is required to meet the standard of SPE Journal. Therefore, my decision for SJ-0823-0080 is major revision.  
  
1) 4D seismic history matching for CCS has been researches by several researchers including the papers as below  
[https://www.earthdoc.org/content/papers/10.3997/2214-4609.20140110](https://urldefense.com/v3/__https:/www.earthdoc.org/content/papers/10.3997/2214-4609.20140110__;!!Bt8fGhp8LhKGRg!Ekv9b_BxMcAiullaniMnZT1QgjK6o7Fq47lRFpm9M6sqLNK76UFib2GLsVZ75TsMj9fzkAivJq9K_WcmHogYbEbpsu9gaKg$)  
[https://www.sciencedirect.com/science/article/abs/pii/S0098300420305963](https://urldefense.com/v3/__https:/www.sciencedirect.com/science/article/abs/pii/S0098300420305963__;!!Bt8fGhp8LhKGRg!Ekv9b_BxMcAiullaniMnZT1QgjK6o7Fq47lRFpm9M6sqLNK76UFib2GLsVZ75TsMj9fzkAivJq9K_WcmHogYbEbp46bokuU$)  
[https://library.seg.org/doi/abs/10.1190/tle36030234.1?journalCode=leedff](https://urldefense.com/v3/__https:/library.seg.org/doi/abs/10.1190/tle36030234.1?journalCode=leedff__;!!Bt8fGhp8LhKGRg!Ekv9b_BxMcAiullaniMnZT1QgjK6o7Fq47lRFpm9M6sqLNK76UFib2GLsVZ75TsMj9fzkAivJq9K_WcmHogYbEbpVePwMzg$)

* Response: Thank you for your comment. We have included these works in our Introduction section.

2) Related to numerical simulation model,  
  
2-1) Was the injection well completed on all 11 layers? If so, what was the reason for not simulating just single layer because the 11 layers have the same properties? Only simulation grids would increase. Also, in case of CO2 injection, the lowest layer is applied for completion.

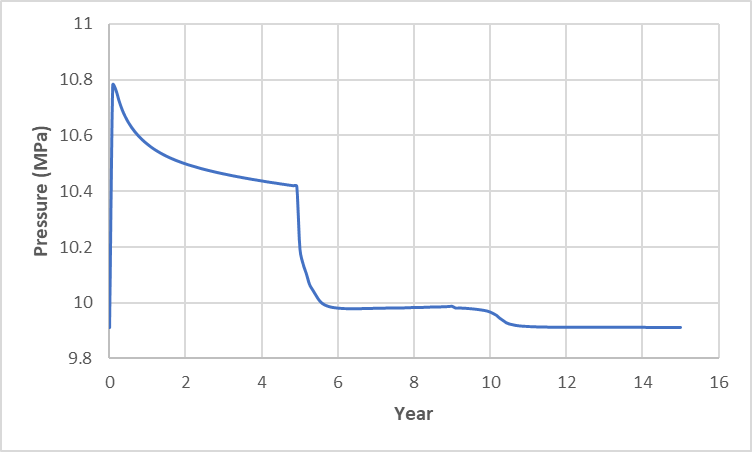
* Response: Yes, we assume the wellbore along the 11 vertical gridblocks is fully completed. We consider 11 layers in vertical direction mainly because we want to let the simulation more closer to realistic scenario including the simulation of buoyancy of CO2 from bottom of injection zone to the top.

2-2) Provide relative permeability curve

* Response: The relative permeability curve we used is the default type for CO2 sequestration simulation in our in-house reservoir simulator FEHM (<https://fehm.lanl.gov/>). The relative curves are linear. Here are the settings for the curve:
  + minimum water saturation (connate water): 0
  + max water saturation: 1
  + water rel perm curve exponent: 1
  + minimun CO2 (l/s single phase) saturation, it is assumed to be l in 3 phase calculation: 0
  + max CO2 (l/s single phase) saturation: 1
  + CO2 (l/s single phase)-water rel perm curve exponent: 1
  + CO2-l CO2-g rel perm curve exponent: 0
  + minimun CO2 (gas phase) saturation: 0
  + max CO2 (gas phase) saturation: 1
  + CO2 (gas phase) rel perm curve exponent: 1

2-3) Provide pressure increase at the end of injection (5 year)

* Response: Thanks for your comment. The figure below shows the pressure chance over time at the injection well based on the simulation results from one of the reservoir realizations. As we can see, the maximum pressure increase at the injection well is less than 1 MPa.



2-4) In Figure 6, it should be clarified that the observed saturation maps were obtained from the reservoir simulation results of ground truth model, not from seismic surveys.

* Response: Thank you for your response. It is true that in this case we have obtained the saturation maps from a reservoir simulator. However, we are under the assumption that these are actually obtained from seismic surveys and converted to saturation maps using a fluid substitution model, as would typically be the case in field applications for GCS monitoring.

2-5) The geological model does not have any anticline structure, which results in minimal changes in CO2 saturation maps between the 15-year and 5-year of the ground truth in Figs. 6 and 7. Therefore, it is meaningless to consider for the 15-year timeframe.

* Response: Thank you for your comment. It is true that there is no anticline structure and therefore the CO2 plume will not migrate vertically (and potentially not migrate drastically horizontally either). However, it is safer to monitor the long-term plume migration for potential leakage risks in monitoring wells, potential changes in CO2 saturation due to dissolution or mineralization, or other potential factors that can affect the long-term storage of the CO2.

3) Related to ES-MDA-GEO,  
  
3-1) Is it correct that for the first assimilation step (the first year) the prior models are updated using ES-MDA-GEO using the saturation map data from the first year, and then, for the second assimilation step (the third year), the updated model are modified again using ES-MDA-GEO using both the first-year and third-year saturation maps?

* Response: Correct. The first assimilation step uses only year 1, while the second assimilation step uses year 3 and year 1. Similarly, the third assimilation step uses year 5, year 3, and year 1.

3-2) If yes for 3-1), please compare the results that ES-MDA-GEO is applied to prior model once using 1, 3, and 5 years saturation maps together.

* Response: Thank you for your comment. The third assimilation step uses years 1, 3, and 5 together, which is shown in Figure 7 (bottom right).

3-3) What is the inflation factor and the number of assimilation step for each assimilation step?

* Response: Thank you for your comment. The total number of assimilation steps is 3 (first is year 1, second is year 1 and 3, third is year 1, 3, and 5). The inflation factors are obtain using the geometric procedure of ES-MDA-GEO, as described in the second paragraph of the Methodology section:

*“a practical approach to determine the precise minimum inflation factor for each data assimilation step. These inflation factors can be obtained through the truncated singular value decomposition (TSVD) of the data sensitivity matrix. By enabling users to set a limit on the total number of data assimilation steps based on available computational resources, this technique offers adequate attenuation of variations in reservoir model realizations during each iteration. This effectively manages overshooting and undershooting, which can otherwise result in crude or imprecise evaluations of uncertain reservoir properties, such as permeability.”*

3-4) How the 3D saturation map data (51x51x11) is used for state vector? Please provide the state vector for the assimilation step 3 (may be 51x51x11 permeability, 51x51x11 1st year saturation,  51x51x11 3rd year saturation, and 51x51x11 5th year saturation).

* Response: The saturation map is used as observational data when we calibrate the reservoir parameters. These data won’t be changed. Only the state vector is updated in order to match with the observational data. The data assimilation workflow designed only outputs the state vector at the final assimilation step. The results for interim steps are not output. However, we can imagine that the state vector (e.g., permeability) is getting closer to the ground truth compared to the state vector obtained in the earlier assimilation steps. This has been observed in many other data assimilation or history matching problems.

4) Related to results,  
  
4-1) In Fig. 5, What is the reason that the 1-year averaged model matched permeability properly even beyond the CO2 area of the ground truth data in Fig. 2? The 1-year averaged model is similar with the updated R1 model at 5-year in Fig. 4.

* Response: Thank you for your comment. On average, the entire ensemble reproduces efficiently the permeability when assimilating year 1, correct. However, beyond the CO2 plume area, the standard deviation is considerably higher than that of the third assimilation step (years 1, 3, and 5). This shows that the third assimilation step is better at updating the permeability distribution as expected.

4-2) Please provide the top and base layers together for Figs. 3, 4, 5, 6, 7, and 9. If there are too many figures in the manuscript, please provide the results of the base layer in the appendix.

* Response: Thank you for your comment. In the first paragraph of the Case Study and Results section, we state the assumption that all 11 layers of each realization share the same permeability distributions. Therefore, the top (1), bottom (11), and in-between layers (2-10), will have the same permeability distributions, and thus seismic survey and saturation distribution.

4-3) In Fig. 8, Please provide the equation for MSE.

* Response: Thank you for your comment. We have included the equation for MSE in Figure 8.

5) Related to data noise,  
  
5-1) Was noise added only to the observed saturation map, or was noise also added to the saturation maps of each model?

* Response: Yes, the noise was added only to the observed saturation map.

5-2) Was the same error set to the measurement data error, Cd, in ES-MDA-GEO as well?

* Response: Yes, we used the measurement data error Cd to quantify the level of data noise.

5-3) When you mention a 10% error, what is the reference point for this 10% error?

* Response: The reference point is the simulated CO2 saturation map based on the ground truth model.

5-4) Regarding the noise, was it assumed to be white noise with specified mean and standard deviation following a normal distribution?

* Response: Yes, the noise is assumed to be a normal distribution. The mean value is zero, while the standard deviations are 1%, 3%, 5%, and 10%, respectively.

6) Related to conclusion, Please compare quantitative metrics like MSE when comparing with previous research (Chen et al., 2020).

* Response: This is great suggestion. Since we didn’t do any comparison in the main body of the paper (not the focus of the paper), thus we thought we should not make that statement in the conclusion. In the revised paper, we have removed the last sentence in the first paragraph of the Conclusions.