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Hydrology and Earth System Sciences
Discussions

Interactive comment on "Probabilistic assessment of field-scale CO_2 generation by Carbonate/Clay Reactions in sedimentary basins" *by* Giulia Ceriotti et al.

Anonymous Referee #1

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The manuscripts provides a showcase for a probabilistic framework at hand of a realistic 3D scenario. The processes under investigation generate CO2 from complex Carbonate/Clay Reactions in deep sedimentary basins where pressures are high and temperatures play a role in fundamental reactive systems. In the following and in the manuscript, these systems are denoted as CCR. As I understand the motivation for this study, it extends previous work of a lower-dimensional concept into full 3D and may be seen as a proof of concept.

We have here a manuscript that falls within the scope of HESS, presents a novel concept with well explained scientific methods. The title is not wrong, but maybe promises

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too much. It is rather a proof of concept for a probabilistic framework, with still a way to go for an 'assessment'. So, I can support this study for publication in HESS, while I have some major concerns, which I am confident can be addressed.

General comments:

I) The research question(s) that guide(s) this work should be formulated more clearly, and be addressed more clearly. I see here two fields where new knowledge is produced, (i) about the probabilistic framework itself, its concept, limitations, applicability, (ii) new insights on CCR and their role in generating CO2 in sedimentary basins (e.g. the statement in Line 295/296 on pressure playing a major role in CCR activation though having minor impact on reaction equilibria). Accordingly, the structure of the manuscript, and in particular the discussion and conclusions should reflect this: in the introduction, in the results, and in the conclusions.

On the physics part, I took home messages like, e.g., pressure matters to build a gas phase, temperature affects equilibrium constants, thus burial depth; or: one CCR is less likely activated while it produces more CO2 than another one. And regarding the probabilistic framework, I am actually not sure what I learned here, see my next point.

II) The probabilistic framework includes some uncertainties (on equilibrium constants) while it takes strong assumptions in many instances. This is acknowledged in the last remarks in the Concluions section. In fact, the list of uncertainties is endless. Understanding even more extended probabilistic frameworks becomes even more difficult, and I fear results get lost in a smoke bomb of probabilistic interpretations. That statement, of course, is exaggerated. But seriously, regarding the classification of uncertainties: first of all, I found it not easy to understand from Abstract and Introduction what the motivation for the "probabilistic assessment" is, i.e. where are the uncertainties. Examples might be given in the Introduction. Otherwise, it takes until Section 3 to find it out. Or in Lines 139-141: my impression is that deciding the mineralogical compositions are uniformly distributed is a strongly simplifying assumption, although

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anything else would only increase complexity, not reliability in any sense. But does this not reduce the informative value of the overall framework, when such crucial statistical uncertainties are neglected.

Therefore: It might be helpful to put the probabilistic framework into a broader context of a clear classification of uncertainties occurring in the application of the framework. E.g. Walker et al. (2003) use definitions of different categories, like determinism, statistical uncertainty, scenario uncertainty, etc. This might help keeping an overview and in interpreting the results.

@article{walker2003, author = {Walker, Warren E and Harremo{\"e}s, Poul and Rotmans, Jan and van der Sluijs, Jeroen P and van Asselt, Marjolein BA and Janssen, Peter and Krayer von Krauss, Martin P}, journal = {{Integrated Assessment}}, number = {1}, pages = {5–17}, publisher = {Taylor \& Francis}, title = {Defining uncertainty: a conceptual basis for uncertainty management in model-based decision support}, volume = {4}, year = {2003}, }

@book{morgan1990, author = {Morgan, Millett G and Henrion, Max}, publisher = {Cambridge University Press}, title = {Uncertainty: A Guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis}, year = {1990}, }

Specific comments:

1) Line 154-155: How should I understand the statement that the equilibrium constant of speciation reactions is the key source of uncertainty? Does this mean a bigger uncertainty than spatial distribution/heterogeneity and choice of CCR? Probably not.

2) Line 213-214: Compatible sounds not wrong and I think, it is absolutely correct to use this wording. The data do not disagree with the model, but what is the message in concluding that the model does not contradict observations? Compatible sounds so weak that it demands for more explanation and interpretation. I am also not sure, but maybe the authors have an idea.

3) Conclusions: Am I right to assume that you suggest for a beneficial application of this framework, the CCR should be known in advance?

4) Conclusions, Lines 411ff: I do not really get the message of this statement. What exactly does âĂŽphysically-based modeling‘ refer to?

Minor comments, typos, etc.:

a) Abstract, Line 3: I was wondering if ’mono-dimensional’ is a known expression. If so, I am Ok.

b) Line 25: ’relatively’

c) Lines 92, 210, and 212: ’formulations’

d) Line 162: it IS always possible

e) Line 312: is depicted (blank missing)

f) Line 401: ’values’

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