Dear authors,
I read carefully your work and I found it a very important contribution in groundwater hydrology.

The methodology is clearly presented, the mathematical background as well. The interpolation part may require some more details but on the other hand it mainly supports the concept.

The results and discussion of the proposed methodology is well presented as well. On the other hand, I have some overall concerns:

1) The proposed method is only digestive for those who have specialized knowledge of the entire tools presented.
2) Please mention the innovation compared to similar works.
3) Most important the presented methodology is very complex to be reproduced. I am not saying that is bad! but there also similar works in the literature that do the same work with a simpler manner. Maybe it would be good, if possible, to have a comparison with one of them. Your method is more detailed but compared to simpler approach the performance is far more efficient? Otherwise, what is the reason to have such many methodological and sometime complex steps.
4) paragraph 2.4 The optimization part needs more details. It is not clear how optimization works here.
5) The proposed 3d methodology consist of inversion, interpolation, optimization. All these steps consider parameters. Therefore, an uncertainty analysis is required to study the uncertainty propagation.
6) How realistic is the upscale of such model to a real case study. I understand the research orientation which is very strong but, this is also a matter of discussion.
7) The fixed parameters of the aquifer model regarding transport it would be good to be accompanied by a sensitivity analysis.