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Manuscript Title: The 3D groundwater salinity distribution and fresh groundwater volumes in the Mekong Delta, Vietnam, inferred from geostatistical analyses

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We would like to thank both reviewers for their time and effort in sharing their comments and suggestions for improvement of the manuscript. These were helpful to clarify some issues, increased the readability and resulted in an improved manuscript.

We will first address the main points that were made by each reviewer (in red font) and propose changes to the manuscript by including updated text / paragraphs (added in green font). Next we address the main textual improvements that were made in the pdf of the manuscript.
All updates are included in the new version of the manuscript, that is attached and named essd-2021-15-manuscript_v2.pdf.

Yours sincerely, on behalf of the co-authors,

Jan Gunnink

Anonymous Referee #1, essd-2021-15-RC1.pdf

Dear Authors,
Please find my comments on your manuscript.
The subject matter fits the aims of the journal.
Overall the quality of the paper is good, data and method are well presented and the results can be used both for groundwater management and further research (i.e. groundwater modelling) in the Mekong area.
➔ *We thank the reviewer for the positive review.*

I agree with the fact that working on delta scale requires assumptions and simplifications.
The biggest assumption that could affect the results and uncertainty associated to all interpolations is the one related to domestic extraction wells, considering the amount of data for each aquifer, especially for aquifer qp2-3 (fig.6). This is my main concern that would require more explanation (see attached pdf).
➔ *With respect to domestic groundwater extractions, the data about the location and aquifer from which the groundwater was extracted were collected during numerous field campaigns over many years that were organized by the DWRPIS (institution at which the second author works). This is reliable data, from which we conclude that at these location fresh groundwater is extracted. We also know that there are numerous extraction wells in the Mekong Delta from which no data is available about the location and depth / aquifer from which the groundwater is extracted. So, unfortunately the latter data on extraction wells cannot be used in the modelling, since we do not know their location and depth / aquifer from which groundwater is extracted. Of course, whenever new data on up till now undocumented domestic extraction wells becomes available, the underlying method is suitable to directly update the model and re-estimate the 3D groundwater salinity distribution and fresh groundwater volumes again. We have added remarks to this effect in the main text, see lines 251-254.*

The appendixes are fundamental to fully understand the methodological approach. There are some parts (i.e. hydrogeological profile in Fig. A1 and formation factor in Appendix B) that I would include in the main text.

➔ *We have included the profile (Fig A1) in the main text as Fig. 3, as we agree that this is indeed needed to understand the hydrogeological build-up of the Mekong Delta. About the Formation Factor, we included a brief summary of Appendix B in the main text (see green text below), and left the more elaborate explanation of how we derived at the Formation Factors in the Appendix. The paragraph now as follows (lines 205-217):*

2.4.2 From borehole-logging to TDS

The intrinsic Formation Factor (F_i) relates the bulk resistivity of a fully saturated granular medium to the fluid resistivity. Archie (1942) defined F_i as the ratio of bulk resistivity over fluid (water) resistivity (ρ_{bulk} / ρ_w) and is valid for clay-free, consolidated sediments. However, the sediments in the Mekong Delta are not clay-free and are unconsolidated, rendering the use of Archie's formula invalid, as discussed by e.g. Huntley (1986) and Worthington (1993). For clayey, unconsolidated sediments, the ratio of bulk resistivity over fluid resistivity is called the apparent Formation Factor, F_a. A modification of the Archie equation is proposed by Huntley (1986) and Worthington (1993) and applied by e.g. Soupios et al. (2007), to obtain F_a. The procedure that was used includes the determination of a lithology-specific relation between ρ_w and $1/F_a$. Groundwater resistivity was determined from an independent dataset relating measured TDS to electrical conductivity of the groundwater. In Appendix B the procedure to obtain F_a is described in detail, and also the validation of the resulting F_i using an independent dataset. The resulting F_i for each lithology is used to convert LN64 to ρ_w.

Uncertainty associated to the interpolations is well explained. The comparison against previous hydrogeological model (Minderhoud et al., 2017) could be improved by given more information about the main differences on drainable porosity and estimate of fresh groundwater volume between the 2 models.

➔ *We added additional explanation in order to clarify the differences between the Minderhoud model and the model in the manuscript, lines 290-292 and lines 631-633. To summarize: the Minderhoud model does **not** include drainable porosity and fresh groundwater volumes, as that model was focused on land subsidence rate projections; these projection do not need drainable porosity as input data. The common denominator in both models is the geometry (base and thickness) of the geohydrological units. The geohydrological model in this manuscript is a more detailed model, based on a much larger amount of data, compared to the Minderhoud model.*

Some important discussion is currently reported in the appendix (C and D), but I would include part of that in the main text.

➔ *We have included a condensed version of Appendix C and D in the main text, and will leave the elaborated version in the appendix. The paragraphs are now as follows (lines 260-286):*

2.4.4 Drainable porosity

To determine the amount of potential extractable groundwater from each aquifer, the spatially distributed drainable porosity is needed. Drainable porosity indicates that part of the total volume of an aquifer that drains under gravity (Fitts, 2002) and is also called effective porosity. It is presented as a volume ratio and thus dimensionless. Data for drainable porosity of aquifers in the MKD are limited. To derive at a spatially differentiated model (2D map) of drainable porosity for each aquifer, each lithological interval in the boreholes was assigned a drainable porosity depending on the characteristics of the sediments, as described in the DWIPRS database. By aggregating over the lithological intervals, an average drainable porosity was calculated at each borehole location within *the aquifer and subsequently interpolated to derive a map of drainable porosity for the entire extent of each aquifer. The procedure is described in detail in Appendix C. The drainable porosity per lithological class is taken from Johnson (1967), see Table 1. The resulting drainable porosity maps are unique, in the sense that previous models of the geohydrology in the MKD either do not model drainable porosity (Minderhoud et al., 2017) or average drainable porosity per province (Bui et al., 2013).*

2.5 Three-dimensional modeling of aquifers and aquitards
To estimate the spatially distributed fresh groundwater volume – including uncertainty – in each aquifer of the MKD, a model of the top and bottom of each hydrogeological unit in the subsurface is required. Minderhoud et al. (2017) constructed – based on 95 boreholes – a hydrogeological model (cell size 1000 x 1000 m^2) of the MKD. The larger dataset used in this study consist of the interpreted base of the hydrogeological units from boreholes and extraction wells (Fig. 4). These were used to update the basic model to a new, more detailed model, by kriging of the base of each unit and consequently stacking the units in the right stratigraphical order to obtain a consistent model. The procedure is described in detail in Appendix D. The resulting layer model was converted into a voxel model (dimensions of the voxel 1000 m x 1000 m x 5 m^3) by assigning the appropriate hydrogeological unit to each voxel. The top of the voxel model was formed by the Digital Elevation Model (DEM), derived from Minderhoud et al. (2017).

The length of the paper looks appropriate considering the complexity of the dataset and methods.

By reading the article and downloading the data set, it would be possible to (re-)use the data set in the future. I am not able to open the two NetCDF files available as dataset, but I am sure it's my fault. I tried with ArcGIS Pro and QGIS, I did not try by python.
➔ *We downloaded the current dataset from the Zenodo website again and were able to import it into ArcGIS Pro.*

Some other small comments and technical correction are reported in the attached revised version of the paper (pdf file).
➔ *Thanks for these suggestions for improvement, we have implemented (almost) all of them.*

Hope this could help in improving the paper.
Best regards

Anonymous Referee #2, essd-2021-15-RC2.pdf

Dear Authors,
I'm a geostatistician with no expertise on groundwater dynamics, then my review is on the geostatistical methods used.
The paper describes the work done to produce datasets on the fresh groundwater volumes in the Mekong Delta. The article is well structured and the presentation is clear and concise. The Figures and Tables complement in an excellent way the text in the manuscript.
➔ *Thank you for your positive remarks.*

As far as I can judge, there are no major flaws in the statistical analysis, though some more work on the text is required. The conclusions are well supported by the results. The accuracy and precision of the results are reasonable and the Authors provide uncertainty estimates of their predictions.

➔ *Thank you again for the positive overall conclusion of your review.*

The presented interpolation method is not original, the Authors state in the Introduction that "To our knowledge, this is the first time that the fresh groundwater volume on a large, delta scale is estimated by means of the geostatistical interpolation technique indicator kriging", which is something I cannot judge.

➔ *Estimating volumes of fresh groundwater for an entire delta by a combination of a detailed hydrogeological model, groundwater quality data (both "hard" and "soft" data) and an estimate of drainable porosity is, to our knowledge, not published before. This also applies to the uncertainty estimates of the freshwater volumes as derived from the geostatistical methods applied. We think that the statement is true; we have reworded it slightly to make it more clear what we mean to say. The paragraph now reads (changes in green), lines 85-91:*

Fresh groundwater volumes for large deltas are not widely available. The employed geostatistical interpolation technique, indicator kriging, provides for each location (x,y,z) the entire probability distribution of TDS and offers the advantage of incorporating data from additional sources. It is preferred over the more often used Ordinary Kriging method when the underlying statistical distribution is departing strongly from a Gaussian (or at least symmetric) model. Besides the delta scale of the TDS estimation, the determination of uncertainty of the fresh groundwater volumes of the individual aquifers of the MKD and the MKD as a whole is unmatched.

The final dataset is publicly available and this is a great merit of the authors.

➔ *Thanks again, we genuinely believe in data-sharing to stimulate re-use of results that are based on datasets that are collected and interpreted at the expenses of society. This also adds transparency to the conclusions and will encourage future research on and management of the fresh groundwater resources in the Mekong Delta.*

It would be great if the authors will regularly update this dataset. They should state more on their future plans in their conclusions.

➔ *We have elaborated on the future plans and use of the model results in the conclusions. For instance, the 3D groundwater salinity distribution will be used in a groundwater study on the effect of sea-level rise and increased projected extraction rates and is the basis for a feasibility study on deep-well aquifer storage and recovery in the province Soc Trang. As also mentioned in response to a remark from the 1st reviewer, we foresee updates of the model when sufficient new data comes available, both "hard" and "soft" data. The added sentences are (lines 503-506):*

The current model can be updated when new data comes available, either from boreholes or information that can be linked to groundwater quality. The calculation workflow is flexible in a sense that data from a range of sources can be incorporated, as long as the data can be reasonable linked to groundwater quality (or drainable porosity).

The study is valuable. My advice to the editor is to consider it for publication after a revision addressing the comments that follow.

➔ *Thank you for the recommendation. In the following the comments are addressed.*

Comments:

I have been able to download from Zenodo and extract data from the netcdf files with tools such as "ncview" and "ncdump". The two files are: hydrogeology_Mekong_Vietnam.nc, TDS_Mekong_Vietnam.nc. The second file contains the two variables: Etype_estimate_TDS, Probability_TDS_smaller_1g_L. The data are made available on grids with horizontal spacing of 1 km and vertical distance of 5 m.

➔ *We are happy to see that it is possible to download and view the model.*

Sec. 2.1. I like Fig.2, very informative. One weak point, it is difficult to link the information in the netcdf files with your description in Sec. 2.1. For instance, from Fig.2 it looks like you are distributing much more data than the variables that are actually present in the files. Please, make explicit the connection between the data presented in Fig.2 and the variables in the files on Zenodo.

➔ *We added some additional explanation in the data availability paragraph (lines 515-526) and we added additional information in in Fig.2 (workflow description).*

Sec. 2.2. This is a rather general description of the methods, where you made the reader aware of the names of the kriging schemes you have decided to use. I agree that ordinary kriging is not well suited for skewed variables. Lines 140-141 are simply wrong, the equation reported has problems with the parentheses and it does not make too much sense to me, because you have not explicitly stated the meaning of "z" with respect to "Z". What does it mean that z is conditional to the number of observations "n"? I can guess its meaning, though I think that you'd better describe this equation or you remove it from the text. (in the first place, is the equation needed?)

➔ *We agree with the reviewer that it is not informative to include this equation in the general description of the methods and therefore have removed it.*

Sec. 2.4. In your study, there is a small number of high quality data, which are presented in Sec 2.4.1, and a much more numerous set of what you call "soft" data. The soft data are unevenly distributed in clusters here and there along the Delta. You implicitly recognize that this unbalance between high and low quality data can introduce bias in your estimates, then the soft data are spatially aggregated. How different is the quality of the estimates from the soft data to those of the high-quality data? I understand that estimates from the soft data rely on some assumptions you make but how good are these assumptions.

➔ *This is a valid point that the reviewer mentions here. The assumption that we made with regard to the quality of the groundwater of the domestic extraction wells is based on the fact that the water is used for domestic purposes and part of these wells were tested by the local authorities or the well-owners to confirm its quality for domestic use. From that we conclude that it is reasonable to assume TDS < 1g/L, the current Vietnam technical regulation guidelines for groundwater quality. For the possible bias this might have on the estimates, please see the answer to the next remark. The TDS for the industrial extraction wells has a lower value, because these wells are thought to be more regulated and some are (unofficially) tested. The local experts have guided us in the selection of these thresholds for TDS, and we added this explanation in the main text (lines 235-237).*

Can the mismatch between different data sources introduce biases in your results? Please, elaborate more on these points.

➔ *Since we are using an indicator approach, in which the data of the domestic wells is only entered for the indicator TDS < 1 g/L, we think that the possible bias for the domestic wells will be small. The indicator < 1 g/L for the domestic wells will influence just that part of the pdf (which is of course an important part) and will not influence the other indicators that constitute the pdf. This is added to the main text (lines 334-340):*

Because the domestic wells represent incomplete data – TDS concentrations are only known to be lower than 1.0 g/L – the indicator coding was performed to take this into account. So, only the indicator that represents the threshold of 1.0 g/L was coded, while the rest of the indicator thresholds were assigned as missing data. This will prevent bias that might arise from using the incomplete domestic well data, since the indicator kriging procedure is informed that only the information about the fact that TDS is < 1 g/L is to be used. This also applies for the industrial extraction wells, in which case the threshold of 0.3 g/L was used.

The unbalance between the small set of high-quality data and the large set of soft data is so massive that the semivariograms are probably determined by your soft data only. This may explain the evident "bull's eye" effects, which are present in Fig.11.

➔ The variograms were calculated from the declustered dataset. Declustering of the high-quality dataset was performed by averaging all the data of TDS in each voxel of 1000 x 1000 x 5m, while the "soft" data was declustered at 5000 x 5000m. So, the possible imbalance in the determination of the variograms is more or less counteracted by the declustering. We have added additional text in paragraph 3.2.2 (lines 350-355):

3.2.2 Estimation of indicator semivariograms

The geostatistical interpolation technique (indicator kriging) calls for semivariogram models for each indicator threshold to estimate the complementary cumulative distribution function of TDS at each location (voxel). The semivariograms were estimated for the median-indicator of the TDS distribution (1 g/L) using the declustered data, in which the smallest horizontal distance between datapoints is 1000 m (horizontal dimension of the voxel). Appendix E describes the procedure for calculating the variograms and the interpretation of the results.

In some regions, where more "soft" observations are present, the fields are reconstructed in a more realistic way. In data sparse regions, red or blue "bubbles" can be seen here and there (see the attached image). Can you comment more on the impact on the inhomogeneities in the spatial data distribution on your results.

➔ The reviewer is indeed pointing out a valid observation, that underlines the importance of the inclusion of the "soft" data. A reason for the discontinuities in TDS is mentioned in Hung et al, 2019. The groundwater salinity distribution can be heterogeneous due to salt water "fingering" processes during paleo times in a heterogeneous geological setting, with sedimentation and erosion cycles. But it is also possible that the inhomogeneities in the data distribution causes these bubbles, especially in data-sparse areas. We added some additional remarks about these phenomena in lines 414-426 (see green text below) and also included the classification of TDS in fresh (> TDS < 1g/L), brackish (TDS 1-3 g/L) and saline (TDS > 1 g/L) in the download of the data. This will give the user a better understanding of the continuity of the groundwater quality for practical purposes. The E-type estimate can be used by for further analysis and modelling of TDS, while the classification into three salinity classes gives an overview of the occurrence of fresh, brackish and saline groundwater in the Delta.

The 3D model of the ccdf of TDS allows for the inspection of the fresh groundwater distribution for each individual aquifer. In Fig. 12 the models of the spatial distribution of TDS are given, again together with the probability of TDS < 1 g/L. In some areas, large variations in TDS are modeled over relatively short distances. One reason might be the occurrence of the so-called salt water "fingering" occurring in a heterogeneous (3D) distribution of lithology that is caused by variable-density groundwater flow during erosion and sedimentation cycles in paleo-times (e.g., Delsman et al., 2014; Larsen et al., 2017; Pham et al., 2019; Zamrsky et al., 2020) . Another reason is that aquifers are incised into sediments that formed aquitards. The modelling of TDS occurred separately in aquifers and aquitards, thereby creating sometimes sharp boundaries in TDS concentration. And in certain areas data sparsity might cause artefacts in the model. The user of the model is reminded that the main aim of this study is to estimate fresh water occurrence and volumes. Therefore, the use of the three classes of salinity (fresh, brackish, saline), together with the probability of TDS < 1g/L (Fig. 11) is valuable for this purpose, while the E-type estimate can be used for further analysis and modelling that requires TDS.

- Sec. 3.2.1. Please move lines 295-299 (discussion on Gaussian transformation) into Sec.2.2.

➔ *Agreed and done*

- Sec. 3.2.1. Lines 283-284 "So, the geostatistical analysis and interpolation of TDS is performed within the volume of each individual aquifer/aquitard by using data that is located within that unit." This is an extremely important information, you should state that your spatial interpolation is performed this way in Sec. 2.2. For instance, by looking at the fields of "Etype_estimate_TDS" in your netcdf files, one can see sharp transitions between different spatial trends. This could probably be explained by this choice you made.

➔ *Thanks for pointing this out. This is indeed an important issue that needs some more attention. In Sec 2.2. we added text to point out that the interpolation is carried out within each separate aquifer and aquitard (lines 148-149: The geostatistical analysis and interpolation of TDS is performed within the volume of each individual aquifer/aquitard by using data that is located within that unit). Furthermore, we added some remarks to point this out to the reader in paragraph 3.2.4. (which is included in the answer to the previous remark of the reviewer, lines 420-422): Another reason is that aquifers are incised into sediments that formed aquitards. The modelling of TDS occurred separately in aquifers and aquitards, thereby creating sometimes sharp boundaries in TDS concentration.*

- Sec. 3.2.2. Please comment on the characteristic horizontal length scales inferred from the semivariogram. Are they comparable to the average distance between your high quality observations? Are they closer to your spatial aggregation of the soft observations? Remember that the real (effective) resolution of the predicted fields are determined by your semivariograms, not by the grid spacing.

➔ *The characteristic horizontal length scales are based on the declustered "hard" data (average of TDS in voxel of 1000x1000x5m). The spatial correlation lengths that are apparent in the semivariograms are therefore not unduly influenced by the spatial aggregation of the (hard and / or soft) data. We added additional explanation in lines 351-353 and in appendix E (lines 658-661): The minimum distance between the declustered datapoints is 1000 m in the horizontal direction. The variograms show a spatial correlation length that is larger than 1000 m, indicating that the horizontal voxelsize is appropriate for the spatial scale considered.*

-Sec. 3. Please make clear to the reader which are the variables that are stored in the netcdf files, by making explicit reference to them when you mention them in the text.

➔ *Agreed and done in the data availability section (lines 515-525):*

Data availability

The downloadable hydrogeological and TDS model, available at https://doi.org/10.5281/zenodo.4441776 (Gunnink et al., 2021), contains the file:

- *"hydrogeology_Mekong_Vietnam.nc" with the variable "hydrogeological_unit", representing aquifers (lowercase) and aquitards (uppercase), with the naming convention according to Fig. 8 and the description in Appendix D.*
- *"TDS_Mekong_Vietnam.nc" which contains the variables:*
  - *"Etype_estimate_TDS", representing TDS concentration (in g/L)*
  - *"Fresh_brackish_saline", in which each voxel is classified as containing fresh (TDS < 1g/L), brackish (TDS 1-3 g/L) or saline groundwater (> 3g/L).*
  - *"Probability_TDS_smaller_1g_L", representing the probability that TDS < 1 g/L.*