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Hydrology and Earth System Sciences
Discussions

Interactive comment on "3D multiple point geostatistical simulation of joint subsurface redox and geological architectures" *by* Rasmus Bødker Madsen et al.

Anonymous Referee #2

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Overview: This paper presents an approach for joint stochastic simulation of subsurface geological and redox architectures in 3D using multiple point geostatistics (MPS). The method is demonstrated on a small catchment in Denmark, where simulations are conditioned on observed resistivities of the subsurface from towed transient electromagnetic measurements (tTEM) as well as on soil maps and borehole observations of lithology, sediment colours and water chemistry.

The paper is interesting and addresses an important topic which fits the scope of HESS. To predict the transport and fate of nitrate and to improve the understanding and management of nitrate contaminated aquifers, detailed knowledge of subsurface

geology and redox conditions is required. The characterisation of the subsurface is usually largely based on borehole data (sometimes together with other ancillary data, knowledge etc.), which subsequently are interpolated to cover the domain of interest. The heterogeneity of the subsurface means that such interpolations can be associated with large uncertainty. Stochastic geostatistical approaches, like the one used by the authors here, are therefore widely used to account for such uncertainties in subsurface mapping and modelling. I'm no expert in MPS or geologist (this is therefore likely to be reflected in my comments below), but to me, it seems appropriate to use the MPS method for the context here, although other methods exist. There is therefore a lot to like about this paper. However, I have number comments and issues that I think should be addressed before this paper can be published. Below are my comments which I hope the authors will find useful. Held og lykke!

General comments:

1. I'm not very familiar with the MPS method and how it works exactly, so I can't really comment on the chosen parametrisation or even on whether the results produced are good/acceptable. However, I do wonder why the simulation artifacts occur? I think this should be elaborated on. It is stated that the geological artifacts are likely due to inconsistencies between TI and conditioning data (L565), but what does that mean exactly? Why do the realisations deviate from the TI? The non-stationarity of the TI is mentioned but I don't understand what this means. It is suggested that artifacts could potentially be removed through better parametrization, but why would that be, and if so, shouldn't you have attempted to do some parameter 'tuning' as part of this work? I understand that the artifacts are basically being averaged out over multiple realisations, and I think if the main aim was to produce best estimate and associated uncertainty (entropy) of the geology and redox (Figure 11), then the occurrence of artifacts would be less of an issue. However, if the aim is also to provide realisations as input for transport and fate modelling of nitrate, then I would think the artifacts could become much more of an issue, especially as flow and solute transport will depend non-linearly on those real-

isations. It is argued that for hydrological modelling at catchment scale, the geological artifacts will have limited effect, which may be true, but I'm less convinced the same is the case for nitrate transport, especially given the redox artifacts.

2. The joint simulation requires a bivariate training image (TI) for geology and redox to be developed. I understand how the geological TIs were developed, but I find it less clear how the redox TIs were produced, who produced them and how the bivariate/joint nature of the TIs are specified. I think this could be better explained.

3. For the case study, two independent bivariate TIs are developed, one representing the Quaternary sequence and one representing the buried valley. It is assumed that the delineation of these geological elements is known in the domain (i.e. no uncertainty as to whether a voxel is Quaternary or buried valley). But what is this delineation based on and with what certainty can this be done?

4. I can't really work out what the influence and significance of the TIs and the conditioning data are for the results. I think it would be relevant to include a discussion on the value of the information used. Given the large amount of conditioning data, does the TI become less important? Would the results be significantly different if you just used the same TI for both the geological elements? What is the effect of the soft data on the result? It would be interesting to see what the results look like if you excluded these. Except for the surface geology, the soft data looks quite uninformative.

5. It is not clear to me exactly how topography is used to inform soil moisture when deriving soft data for redox conditions. L365 just states how slope/topography affect moisture in general (it sounds like a TOPMODEL type of approach?). I think further explanation is required here.

6. Figures: The 3D figures look impressive, but there is a lot of them, and I think they are quite complex, and the colour choices make them not so easy to 'read' (especially the small ones). I wonder if some of the figures would perhaps be more illustrative in 2D rather than 3D. I don't think Fig 5 works very well as a 3D figure, and in Fig. 6 it

is difficult to see that tTEM actually only covers part of the simulation grid. In Figure 1a it took me a while before I realised that the blue, black and red lines where actually the TEM and ERT data points. In Figure 7 the colours are difficult to distinguish in the histograms and it looks like there is a shade of blue in Fig 7a that is not in the legend.

7. Overall, I think the paper is well-written, but there are places where I find the presentation of the material unclear and confusing and where more explanation would be helpful (particularly section 6 and 7). I appreciate that this is not helped by the fact that I'm not so familiar with the MPS method.

Minor specific comments:

Abstract: I struggled to understand L16-22 when reading the abstract the first time around (and the similar paragraph in the introduction, L106-110). It makes more sense to me after reading the paper, but I would encourage the authors to sharpen the text here.

Figure 1c: Are the white areas unknown soils?

L167: Rephrase. It sounds like you are doing hydrological simulations as part of this work, which you are not.

L169: There are 7 classes Table 1.

L199: Not sure I understand why they provide independent measurements of redox.

L255: consists of. . .

L306: From figure 1 It looks like the data availability is better in the southernmost part of the domain?

L310-311: I do not follow this. Why is sandy till not included in the TI? How does that affect simulations for the buried valley and can simulations here then meaningfully be conditioned to observations of sandy till?

L313: I'm not sure I understand what you mean by translating the geological TI to a redox TI by integrating geochemical and water chemistry data. Is the redox TI mainly based on the geological TI, e.g. redox conditions are generally reducing in (upper) areas with meltwater sand, oxic at surface near sediments etc.? And then just making some adjustments based on measured data? That's almost how it looks from Figure 4.

L321: I don't understand how its eases the construction of the TI to include parts outside the domain. Please clarify.

P16 and Fig 7: I find it difficult to follow the text and observations that go with Fig 7. It is stated that sandy till is associated with some of the highest resistivities, but I can't see this from Fig 7. I don't follow how the general relationship /distribution of resistivities have been derived (Fig 7c). I think this whole section could be clearer.

Equation 2: I'm not sure I follow the equation. Is the soil map (surface geology data) used to inform the lithology below the surface layer as well in a similar way as in the buffer zones as described in section 5.4.2? Or what is the probability of surface geology below the surface layer (intuitively I would think zero probability in which case the equation collapses)?

L435: . . .overlapping relationship. . .

Soft data: do you derive soft probabilities for geology for all voxels in the simulation grid, even where hard data are present? It looks so from Fig 8 and 9.

L457: To what extent did you experience "flagging" as part of the simulations you generated?

L485-500: I found some of the described observations here difficult to see in Figure 10. Maybe it would be easier to follow if there was a close-up on a relevant part of the transects instead?

L555: I'm not sure I understand why and when your simulations would not honour TI and data.

L574-585: I think the text here reads so well and it could be improved. This is also where terms like stationary TI and rotation in simulation are mentioned, which I find difficult to really follow not having a MPS background.

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