Hydrol. Earth Syst. Sci. Discuss.,
https://doi.org/10.5194/hess-2020-444-RC1, 2020

Hydrology and Earth System Sciences Discussions
Open Access

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

Donald A. Keefer (Referee)

dkeefer@illinois.edu

Received and published: 24 October 2020

This manuscript is included for consideration of a special issue: Frontiers in the application of Bayesian approaches in water quality modeling. It is important to note that the research described in this manuscript does not use Bayesian methods, and so does not directly relate to the topic of the special issue.

Leaching of agriculturally-applied nitrogen is a significant threat to global groundwater resources. Success in reducing nitrate contamination in groundwaters by modification of farming practices and reductions in fertilizer input has been only occasionally realized and more work is definitely needed. Prediction of the fate and transport of fertilizer-based nitrate is a complicated problem that is confounding successful remediations to the groundwater contamination problem. Modeling success is significantly limited by the natural heterogeneities and complexities of the subsurface geologic systems and by our limitations in characterizing and modeling those complexities. The complex nature of the heterogeneities has led to the treatment of these systems as stochastic which has subsequently led to a large interest in probabilistic modeling approaches.

Multiple Point Statistics (MPS) has proven to be an innovative and successful probabilistic approach to modeling inter-facies relationships, primarily within distinct, lithostratigraphic units. As typically used, MPS is not a method that can be used with stratigraphic units or with units that are genetically distinct (e.g., from subglacial environments and glaciofluvial environments), unless each genetically-distinct succession is modeled within separate portions of the model domain. To my knowledge, a modified MPS approach has not been successfully applied to modeling of larger stratigraphic assemblages of rocks or sediments. It would be particularly relevant and innovative if the authors were to present a method for adapting MPS to stratigraphic unit modeling. They do not suggest they are doing that here.

The authors have done a great job in selecting a globally-significant problem to study. They are also commended for their innovation in wanting to pair joint modeling of geology and redox conditions through MPS methods. In terms of formal review criteria, the scientific significance of this manuscript is ‘good’ to ‘excellent’. The overall presentation is inconsistent, making the presentation quality ‘fair’. Some parts are well written and logically argued, but there several important places in the text need more clarity or better explanations. There are a few key places where critical description of methods are missing. The graphics are of good quality and well chosen. However, given the small size and high complexity of the models, the color differences in the geologic models are difficult to interpret. The captions often need to be improved; they need clearer descriptions of what is actually shown in each figure. Importantly, however, I have significant concerns about the scientific quality of key aspects of the study design. Specifically, decisions about the representation of the geology, application of the geologic representation to the MPS modeling approach, and the discussion of the modeling results are all ‘fair’ to ‘poor’. These scientific quality issues are addressed in detail, below. Overall, I believe this manuscript requires significant revisions prior to publication, but that if these concerns are addressed, it clearly merits another review opportunity.

The primary problem I see with the scientific quality in this manuscript is that the geologic deposits are represented as simply a succession of distinct textures (i.e., facies), when the depositional origin, size, distribution, and description, suggest the deposits being modeled are a succession of stratigraphic units, with similar textures, that were deposited through an unspecified number of distinct ice events. MPS would be a clearly suitable approach if the authors were modeling textural distributions within the meltwater sand/gravel and clay/silt assemblages, or modeling the distribution of textural facies or inclusions of sorted sediments within the till deposits. However, in that situation, they would have to model the main deposit boundaries separately (using some other approach) and later insert the textural simulation results into each main deposit. Instead, the authors are trying to apply MPS to a collection of sediments from two or three distinct depositional environments (i.e., subglacial, proglacial fluvial, and maybe proglacial lacustrine), and from 2-4 distinct ice events.

This is more than just a conceptual problem. The MPS algorithms use the training image to guide the location of textures, but every texture has a non-zero probability of occurring anywhere in the model domain. This is not problematic when the facies are all generated within one, single depositional environment. It is problematic when the facies are from multiple depositional environments (and from multiple ice events). Operationally, this matters because under this latter scenario, the realizations can be expected to have sediments from depositional environments and ice events that are randomly out of sequence. Post-glacial sediments can be expected in many subsurface locations. Too much meltwater sediment should be expected within the upper clay till unit. Too much clay and sandy tills would be modeled within the meltwater succession. Since till units are typically associated with distinct ice events, the clay till will be modeled in too many (and maybe occasionally too few) sedimentologic positions to be consistent with the geologic history. This also means that your geologic framework will lead to parameterized groundwater models with predictably-incorrect patterns of hydraulic heterogeneity – one of the main things MPS is trying to avoid. While the distributions of units in the valley-fill (Northern buried valley) setting are a bit more complex, for the same reasons this setting appears to be better described as a succession of stratigraphic units. As with the upland succession, modeling subglacial and proglacial deposits as facies within a single zone is particularly problematic with MPS. In a complex valley fill succession that is composed of multiple erosional/depositional events, it can be very difficult to see the resulting biases – you are expecting complex assemblages and complex assemblages is what you get. The logic of the model doesn't change, however, and the errors for the upland will inevitably be carried over to the valley deposits.

I noted early in my comments that the presentation quality of this manuscript is not ideal. It is possible that I have misunderstood the geologic setting and the approach taken to configure the MPS in this study. However, the description of the geologic deposits does not provide enough clarity to understand the geologic history of the model domain, or the consequent distribution of stratigraphic units and sediment textures. The authors also do not acknowledge this important geologic constraint to the successful application of MPS, nor do they provide discussions on their rationale for using MPS in this setting or on the design targets for texture proportion and zonation. This prevents a clear understanding of what the geologic history is known to be, and how this modeling approach is being used to reliably model the sediment while using that knowledge as a necessary constraint.

My last comment regarding the poor scientific quality addresses the poor quality of sim-

Printer-friendly version

Discussion paper

ulation results for the geologic deposits. Based on the figures of the model realizations and from one or two oblique comments from the authors, these results appear to have an unacceptable fit with the data and training images. The authors barely note the quality of fit in their discussion and (except for a reference to unspecified algorithmic artifacts that generate occasional small errors) they do not provide sufficient technical explanation of why the simulation results fit so poorly with the geology training images. More importantly, the authors suggest that they could have made the solutions better fit the training images, but stopped with the simulations so they could present the method as a viable option. This needs to be fixed prior to submitting a methods manuscript for publication. Until an author can demonstrate clearly and objectively that they can reliably meet the stated modeling goals using the proposed method, the method is not ready for publication.

Acknowledging these limitations within the manuscript, the authors are encouraged to fix these issues, remodel the area, and revise the manuscript. If these issues are corrected, this manuscript would be a worthwhile contribution to the literature.

Interactive comment on Hydrol. Earth Syst. Sci. Discuss., https://doi.org/10.5194/hess-2020-444, 2020.