

Response to Reviewer #1

We are thankful to Reviewer #1 for his/her valuable comments and suggestions, which certainly improved the manuscript. The response to the individual comments is given below. The original review is quoted in *italics*, whereas our response is given in **bold** font.

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This manuscript is a well-written and clear case study on the application of MPS to a very large domain. As such, it will be valuable for a range of researchers. While I recommend eventual publication, I also have reservations that should be addressed.

10 *Regarding the content of the study, I appreciate the overall methodology and the emphasis, throughout the discussions, on the fact that the training image and the simulation algorithm are all elements structuring the final models, and as such the evaluation should take place on unconditional realizations.*

However, I also found that the conclusions would be much better supported by adding a few elements:

15 *1) Currently only a single realization is used for each setting. This is clearly insufficient. On top of p. 12 it is argued that the simulation is considered representative, however I don't agree with this statement. Multiple realizations are needed to quantify uncertainty. It is possible that the single realization is representative, but the only way to find out is to compare with a set of other realizations and decide whether the inter-realization variability is small enough, according to a given criterion (e.g. flow, transport, etc). On p.12 (l.11-12) it is also argued that the methods to use multiple realizations do not exist, which is clearly not the case.*

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Concerning the representativeness of the realization discussed in our manuscript, it is possible to state that, by definition, each individual realization is representative. In fact, every realization is, by construction, compatible with all the input information (i.e., the statistics formalized by the training image, the hard data, and the soft conditioning). In the new version of the manuscript, we added a few lines stressing on this, very important, aspect.

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Concerning the uncertainty assessment, even if it would be definitely very interesting in principle, we feel it would be out of the scope of the present research that is solely dealing with the development of the optimal strategies for conditioning the simulation and for preparing effective training images.

30 *2) The assessment of the results is mostly qualitative, both regarding the patterns produced in the model, and to assess the proportions variability (top of p.8, top of p.9). The tools to do exist and should be used. Also, quantitative comparison of the modeled patterns and the patterns in the conditioning data would be a good validation.*

With respect to a quantitative analysis of the proportions variability, we think that our point (i.e.: the kriged sand probability is effective in enforcing the proper spatial trend) is clearly shown by the comparison between Fig. 17b (in the new version) and Fig. 8. In fact, the two figures allow a voxel-by-voxel comparison between the soft conditioning distribution and the final corresponding realization. However, in order to meet the reviewer's request, we added, in the new manuscript, Fig. 18 showing the cross-correlations between the soft probability distribution (Fig. 8) and each of the realizations (c) and (d) in Table 1 (and plotted, for example, in Fig. 14c and Fig. 14d).

Regarding the quantitative assessment of the produced patterns, we believe that the comparison of Figs. 10a and 10b, showing the unconstrained realizations associated with the training images TI1 and TI2 (in Figs. 9a and 9b respectively), demonstrates quite well the large effects on the final realizations caused by relatively small perturbations in the used training image. But, in order to make our point clearer, we included in the revised version, three more figures: Fig. 11 (showing the sizes of the connected sand bodies for, respectively, the unconstrained realization generated by TI1 and TI2); Fig. 12 (comparing the eccentricities of the unconstrained realization for TI1 and TI2); Fig. 13 (demonstrating that the connected bodies for the unconstrained realization associated with TI1 are more jagged than the others).

3) The literature review part of the introduction is quite incomplete, missing a number of studies that have looked into 3D MPS models. On p.2 l. 25 it is said that not many studies have looked at 3D TI-based models. I disagree, with for example Ronayne et al (2008), Jha et al (2014), Perez et al (2014) to name a few, and a lot of other studies in reservoir engineering as well. For non-stationarity also, there are Cuhgunova et al (2008), Straubhaar et al (2011), and possibly others, who made important contributions.

We acknowledge the relevance of the suggested studies. In the revised version of the manuscript, we included the additional references.

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Regarding the structure of the document, I also have 2 remarks:

1) There is an imbalance between the description of the data and methods, which is quite short (6 pages), and the discussion/conclusion, which is 5 pages. There is clearly too much material in the discussion, including elements that could be removed or moved to other sections. Here are some suggestions:

30 - P.7, l.15-20: this could go in section 5.4.

The rationale behind our original choice is that, in the initial part, we wish to simply present the different inputs and how we used/prepare them.

In the second part (from paragraph “6. Results”), we show the effects of the choices we made and the reasons for these choices. We do this by means of a detailed discussion of the corresponding results.

So, even if it might seem unbalanced in terms of length of the different parts, we believe that, in this way, the paper is more effectively organized from a logical point of view, with a clear separation between the inputs (and their preparation) and the outputs (and the associated assumptions/choices).

- P.9, from l.19: this could go in the introduction

The same concept is already in the “Introduction” and it is (re)discussed in the “Discussion” only for sake of clarity.

- P.10, l.22 to p.11, l. 2: This is not related to the purpose of the paper and could be removed.

Following one of the original suggestions of the Editor, we added this part to reinforce the discussion on the possible use of seismics via the comparison between the characteristics of the seismic lines collected in this area with those acquired somewhere else for hydrostratigraphic studies.

- P.11, l.3-10: The method for the conversion of boreholes to probabilities should be described in the methodology section, not here.

The conversion of the borehole into probability is indeed discussed in the “5.3 Borehole data” section, where we describe the methodology we use to prepare the inputs. In the section “7 Discussion”, we simply recall that strategy to mention possible, straightforward extensions of the presented approach, for example, to the case where boreholes have varying quality.

- P.11, l.11-19: There could be a separate section on non-stationarity because it is mentioned often.

Non-stationarity is tackled by kriging the probability derived from the boreholes. For this reason, we think it is more logical to keep this aspect tightly connected (across the entire paper) with the discussion about the borehole data and the sand probability spatial trend.

- P.11, l.20-34: This is a long paragraph on something that is not done. It could be removed.

Actually, we believe that a discussion on why we made the choice of not to do/show something could be relevant for the community and can contribute to the overall clarity and usefulness of the manuscript.

2) Sections 2, 3 and 4 could be grouped together as they all relate to the description of the study site.

5 In the original and new manuscripts, for expositive clarity and logical sequentiality, we decided to keep these sections separate in order to maintain well distinct:

- i) the prior overall geological understanding of the entire area,
- ii) the observed and utilized data (seismics and boreholes), and
- iii) the description of the specific geological unit to be investigated (the Miocene) .

10 *Other remark:*

Figures 7 and 8: the green-purple color scale is very subjective and seems to highlight values around 0.4. It creates artificial discontinuities. A usual continuous color scale (rainbow or grayscale) would be better.

15 This specific color scale has been selected because 40% is the target marginal distribution value (as it has been derived from the boreholes, and as it is consistently formalized in the training images). The details for this choice are described in the methodological section “5.3 Borehole data” where we discuss our approach for dealing with borehole uncertainty and for translating the lithological information into probability. For these reasons, we believe that the adopted color scale is not subjective and the value 0.4 has a specific meaning as it corresponds to “no information” about the occurrence of sand or clay.

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Response to Reviewer #2 comments

We thank Reviewer #2 for taking the time to review this paper. We sincerely appreciate his/her insightful and constructive comments and suggestions. The response to the individual comments is given below. The original review is quoted in *italics*, whereas our response is given in **bold** font.

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This paper presents a case study of multiple-point statistical simulation of sand/clay occurrence. The paper focuses on two aspects of multiple-point statistics: (1) 3D training image development and (2) different conditioning strategies to incorporate borehole data and geophysical data. This is a very relevant topic. Especially the construction of 3D training images is indeed still difficult. There are definitely some very interesting ideas in this paper, such as the different ways of

10 *using borehole data as hard or soft conditioning data. I would like to see, however, some more discussion on the following points:*

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In the title and aims of the paper, the authors stress the importance of realistic 3D training images. They write that they present a workflow to build a training image. The part about how they build the training image (section 5.4) is however very short. From this short description, it is not clear to me how exactly the training image was constructed. On what data is the TI based? On seismics or on the existing Miocene model? How were the shapes/geometry/position of the clay/sand features determined? What was the input in the Geoscene3D model? How exactly does this model work? What are the assumptions? Is this a manual or an automatic method? What are the “interpretation points” and where do they come from? They refer to a methodology in an earlier paper, but this paper uses completely different input data, i.e., airborne EM data?

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On page 7, the authors write that “the results are evaluated and compared against the structures expected from the Miocene model”? How exactly? Was this model not already used as a basis for the TI? Is it then fair to use it again to evaluate the resulting structures?

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In the new version of the manuscript, the TI characteristics and the details of the strategy we have used during the TI development are provided in the extended section “5.4 Training image”, and discussed thorough Figs 9, 10, 11, 12, and 13. Along the paper, we emphasize the importance of unconditional realizations to assess the quality of the selected TI (actually, in combination with the used simulation algorithm). As it is shown by the comparison in the original Fig. 10, and in the new Figs 11, 12, and 13, even small perturbations in the TIs (Fig. 9) affect significantly the

30 **associated realizations.**

Moreover, in the new version of the paper, we added further details to the description of the TI construction: The first TI test was based on the existing 3D geological model (the Tønder model) covering an adjacent area. This first TI attempt was then manually adjusted during several iterations based on the unconditional output (in the paper, for simplicity, only the initial and final TIs are shown). This iterative process stopped when the corresponding

unconstrained realization was found satisfactory in terms of its ability to mimic the geological features we expect in the Miocene, across the study area. Those expectations about the geology are based on our prior geological understanding of the area, the available seismic lines, and the few existing deep boreholes. The entire procedure is manual (except, of course, the unconstrained simulation).

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Regarding the “interpretation points”, they relate to the interpretation of the geophysical data and the consequent construction of the associated (manual) 3D geological models (as described in Kristensen et al., 2015 and, shortly, in Fig. 5 in the manuscript). In the presented workflow, in particular, they are used, within Geoscene3D, to efficiently modify the TIs. In fact, the interpretation points define the surfaces delineating the volumes to be populated with, for example, sand/clay voxels. By manually changing their locations and creating/deleting some of them, we could have a full control over the adjustments of the TIs. In order to make this point clearer, in the revised version, we added few lines with a short explanation on the use of the “interpretation” points for the TI construction.

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Jørgensen et al., 2013 is mentioned simply as an example of research performed by using the voxel modelling tools available in Geoscene3D and specifically designed for (manual) 3D geological modelling.

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The simulated structures are relatively simple and uniform. Is it really necessary to use MPS? If you would model sand/clay occurrence with a more simple method such as indicator kriging, you would probably get similar results? It would strengthen the paper if you can prove somehow that this relatively complex approach has significant advantages over simpler approaches.

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We showed that even small details, which seem to be “irrelevant” in the TIs (that are capturing the available statistical information regarding the object to simulate), have actually significant impacts on the results (old Figs 9, 10, and new Figs 11, 12, and 13).

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Moreover, this is not meant to be a paper about the comparison of the performances of MPS as a tool to incorporate complex statistical information against other “simpler” approaches. This manuscript deals with the optimal strategies (within the MPS framework) to include the available data into the simulation as soft/hard conditioning, and to build the most (geologically) effective TIs.

As a matter of fact, however, we believe that MPS’ strength lies also in being quite intuitive: for many users, it is difficult to apply (and deeply understand), for example, indicator kriging and properly choose variogram models, while MPS allows the geologist to provide complex information in form of TIs, which is clearly a more intuitive (and, at same time, generally, a more effective) approach.

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More in general, the conclusions of the paper are only based on visual inspection of the simulated clay/sand patterns. There is not objective or quantitative way of comparing the different results. For example in Figure 11: could you not use cross-

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validation or something similar to come to a more objective comparison of the different realizations? I also wonder how relevant the differences between the different realizations are, e.g. when you state that “the realizations showed a significant sensitivity to the TI”. If you put these different realizations in a groundwater flow model, it is quite plausible that they all give similar results. It would be really interesting to using your geological model for some flow runs to see whether the
5 different realizations based on different conditioning strategies really result in different groundwater flow patterns.

We agree that, in principle, it would be very interesting to investigate the results of flow models based on the different realizations. However, we feel that this would be out of the scope of the paper. Adding this kind of considerations would probably make the discussion lengthy and distract the reader from the main focuses of the paper, that are: 1)
10 how to include, in the most effective way, the available data as simulation conditioning, and 2) how to build a TI that is capable to reproduce the geological features we want to see in the realizations. In particular, regarding the latter point, the ability to generate meaningful geological realizations should be seen in a general perspective and, so, relevant per se. Hence, even if, in this specific case, the differences between the two realizations in Fig 10 might be not “significant” for a flow model, the geological differences are evident, and, in principle, could impact the by-products
15 generated by using the realizations. This paper is about the optimal practices to prepare the best possible stochastic geological inputs for subsequent applications.

Concerning quantitative analyses of the different realizations across the paper, regarding the two realizations in Fig. 10, in the new manuscript, we added three more figures showing the distributions of the size, eccentricity, and
20 jaggedness of the connected sand bodies.

In general, with respect to a quantitative analysis of the proportions variability of the different realizations discussed across the paper, we think that our point (i.e.: the kriged sand probability is effective in enforcing the proper spatial trend) is clearly demonstrated by the comparison between Fig 17b and Fig. 8. The two figures allow a voxel-by-voxel comparison between the soft conditioning distribution (derived from the boreholes) and the final corresponding
25 realization. However, following the reviewer’s suggestion, we calculated the cross-correlation between the kriged sand probability (Fig. 8) and the realizations (c) and (d) in Table 1 (and showed, for example, in the new version, in Fig. 14c and Fig. 14d). Not surprisingly, the correlation with the realization (d) has a much pronounced and higher maximum.

30 *The authors claim that in the study area many of the borehole records are of low quality. Why is that? In what sense are they of low quality? How can users in other study areas determine the quality of boreholes and decide whether they can treat the borehole data as hard or soft data?*

Boreholes, like any other kinds of data, are affected by uncertainty. The level of uncertainty determines the quality/reliability of the measurements (i.e., the quality/reliability of the boreholes). Many factors impact the quality of boreholes. Just to mention a few of them: (i) the drilling methods (e.g.: rotary drilling and air lift drillings. In some cases, for example, the finer sediments can be flushed out and the driller could potentially misinterpret, as more sandy, a clay layer); (ii) the drilling purpose (sometimes, if the goal is to reach a specific target, the lithological description can be poor since it is not a priority); (iii) the age of the boreholes (for example, nowadays, in Denmark, samples are collected systematically every meter, and this was not the case few years ago); (iv) the presence of simultaneous wireline logging data (these kinds of ancillary information make the geological interpretation definitely more certain). During the initial phases of a standard geological modelling, a skilled geologist goes through all the borehole records and verifies all these different pieces of information and check for inconsistencies.

In the paper, we mentioned that, for example, we use the seismic data as hard data because they were considered highly reliable and the scale of the structures they were able to delineate was comparable to the scale of the simulated outputs. Clearly, this is not true for the boreholes.

For sake of completeness, following the reviewer's request, we decided to add, to the new version of the paper, few lines to clarify how the borehole data should be, at least in principle, evaluated and prepared for geological modelling.

The results of the paper are based on visual comparisons of individual realizations using different conditioning strategies. It would be really interesting to see multiple realizations for each conditioning strategy to see the variability and uncertainty of different realizations.

We agree with the reviewer that investigating the variability and uncertainty would be interesting. However, we believe that this would be out of the scope of the present paper.

On page 9, the authors write that realization rarely have the same spatial variability as the training image. I find this a really strange statement. The idea of MPS is that you produce realizations with similar spatial patterns as the TI. If the realizations do not show similar patterns, this usually means that the parameters have not been chosen optimally or that the TI was for example not large enough. They also claim that therefore a TI should be chosen together with a specific MPS algorithm? I find this really strange. In my experience, all MPS algorithms can produce realizations with similar patterns to the TI given that they are used in the right way. If the authors really want to claim that different MPS algorithms have different capabilities in reproducing patterns, they should show a comparison of the different algorithms.

The meaning of what we wrote in section “7 Discussion” concerns the fact that, while, ideally, the effects of the TI should not depend on the algorithm choice, these is not true in practice. The different implementations, and the

different parameters that can be tuned during the simulation, make the realizations algorithm-dependent. It would not make much sense to compare the realizations generated with different algorithms, not only because different algorithms have different parameters to be set, but also because the point of the paper is that the TI must be developed, no matter what, by studying the unconstrained realization and its accordance with our geological expectations.

Basically, we claim that the TI and the simulation algorithm are all interdependent elements structuring the final models, and, as such, the evaluation should take place a-posteriori on unconditional realizations.

On page 12, the authors write that “probabilistic models need to be developed and refined in order to utilize the multiple realizations and the uncertainty they represent”. There are however many methods available and applications of MPS using multiple realizations to assess the uncertainty. The methods to do this are available but the authors have chosen to work with single realizations.

Writing that, we meant that applications and methods that are making use of the full potential (for example for geological modelling) of probabilistic models (with their large number of realizations and information regarding the uncertainty) are still under development. Those lines in the original manuscript were not about the possibility to assess the uncertainty via analyzing the realization ensemble.

The reasons why we decided not to investigate the uncertainty are largely discussed before in the present document.

The paper is clear and well written. The figures are of good quality.

P4, line 24-25: “along extended profile”: error in grammar of sentence?

We thank once more the reviewer for the positive comments, especially because we invested a lot of time in the preparation of good quality, and, hopefully, clear, figures.

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We believe that “along extended profile” reflects what we mean.

Response to Referee #3 comments

We thank Referee #3 for his/her valuable comments and suggestions. The response to the individual comments is given in the following. The original review is quoted in *italics*, whereas the response of the authors is given in **bold** font.

5 *Multiple-point simulation (MPS) is a geostatistical simulation technique first developed at Stanford University in the early 2000's. An MPS algorithm is used to reproduce spatial patterns, such as connectivity, that are depicted in a training image (TI), which contains the possible spatial configurations for any given geological object and relationships between objects. A TI contains only spatial patterns and their respective likelihoods. A frequent pattern appears more often in the TI than a rare one. The actual position of a pattern in the TI is largely irrelevant, the MPS algorithm sees a set of patterns and tries to set*
10 *them together through a randomization process. In order for an MPS simulation to produce a reasonable representation of any given geological system, it must have to honor some conditioning data and have a method of accounting for spatial trends in the probabilities of selecting patterns from the TI.*

The title of this paper suggests that, in this case, these MPS simulations are to guide subsequent hydrogeological applications. The title also suggests the main thrust of the paper is the importance of developing realistic 3-D TI's and strategies for conditioning MPS models. However, this topic is only discussed rather briefly (in 10 lines) in section 5.4 on page 7!

In the new manuscript, the TI characteristics and the details of the strategy we have used during the TI development
20 **are provided in the extended section “5.4 Training image”. Moreover, they are discussed thorough Figs 9, 10, 11, 12, and 13. Besides, along the paper, we repeatedly emphasise the importance of unconditional realizations to assess the quality of the selected TI (in combination with the used simulation algorithm).**

We believe that, in the new form of the paper, the iterative strategy we developed for the optimal construction of the TI is sufficiently clear.

25 **Regarding the conditioning strategies, they are discussed throughout the entire manuscript.**

In the first place, they are introduced in the methodological section “5 Defining MPS input information”. For example, sections “5.1 Seismic data” and “5.2 Existing 3D model” are devoted to the reasons for using the seismic data and the boundaries of the pre-existing geological model as hard conditioning, while section “5.3 Borehole data”
30 **describes how to translate boreholes into soft conditioning data by means of a moving window approach and discusses the importance of kriging the “localized” borehole information to enforce the necessary spatial trend.**

The results of the application of the different conditioning strategies - introduced in the section “5 Defining MPS input information” - are then compared in section “6 Results”.

Section “7 Discussion” examines the assumptions and choices we made and the future possible developments of the presented conditioning strategies and TI development workflow.

So, a large portion of the manuscript is devoted to the detailed descriptions of the optimal approaches for conditioning and TI construction, which are the focus of the present study.

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I thus found the paper rather confusing and yet I recognize that the authors and their organizations have considerable experience in 3-D geological modeling for hydrogeological applications, and that there is a considerable body of observational data in southern Denmark that can support the development of multiple-point simulations of the subsurface environment.

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In short, while individual sentences and paragraphs use consistently good English, I became uncertain about many important details of their research and objectives. The paper is quite lengthy in its current form, yet it leaves many questions unanswered. In fact, I believe the paper raises more questions than it answers.

15 *I therefore propose that, for publication, the authors undertake to reorganize the current text into something similar to the following:*

Section 1: Introduction: This should clearly define the background, objectives, a scope of this project. These topics, I believe, include: “A desire to evaluate the Miocene sediments over a 2810 sq.km. area of southern Denmark where they provide the source of most drinking water. “For about 22% of the area, there is a detailed 3-D stratigraphic model (lithostratigraphic and/or hydrostratigraphic?) developed by deterministic methods (the Tonder model) “Southern Denmark has some high-resolution seismic surveys that can be used as conditioning data for MPS simulations (However, the authors need to provide more information about the spatial adequacy of these surveys, not just that they total 170 km and are shown (rather poorly) on Figure1). “While existing borehole records are available, they are of relatively low quality (WHY?) and most borehole are relatively shallow, so these can provide only limited-value conditioning data. “The project was undertaken to determine if MPS could produce 3-D subsurface information over the entire southern Denmark area more efficiently than deterministic modeling, yet still produce information of value to further hydrogeological models.

20 *Section 2: The Study Area and Available Data Sources: This should summarize its geological character and assess the various data sources. This can be accomplished by revising as necessary existing sections 2 and 3 and Figures 1-5. A discussion about trends should be enhanced.*

25 *Section 3: The Experimental Process. This needs considerable expansion from existing section 4. Several questions arise from reading the existing paper. Chief among them: Was the Tonder model the source used to develop the TI? Currently this is unclear. Later the use of two TI's is noted. How were they developed/selected? What are the spatial characteristic patterns desired in the TI?*

Section 4: Analysis of Results. This will combine information from existing sections 5 and 6 and some of 7. It also should address several of the limitations defined below.

Section 5: Discussion and Conclusions. This should be relatively short, but include some of the ideas in existing sections 7 and 8. It also should address the need to determine what level of subsurface detail is required to produce an acceptable groundwater management tool for regional and more site-specific applications in southern Denmark (see my final comments).

We arranged the paper as follows:

- 10 1) **“1 Introduction”** - the first section after the abstract - is devoted to a very general and brief discussion of the existing literature on MPS.
- 2) **The second section “2 Study area”** deals with the overall geological framework of the area. So, this section delineates the general geological setting where the unit investigated in the paper (the Miocene) is embedded. This, at the same time, contextualizes the presented research and better defines its limits.
- 15 3) **Section “3 Data”** describes in detail the amount and characteristics of the different kinds of data available (borehole data and seismic measurements). In particular, a large part of the paragraph “3.2 High-resolution seismic data” discusses - to a reasonable level of detail for the purpose of the present study - the different specifications of the seismic data available.
- 4) **Section “4 Establishing framework-model constraints”** goes into details about the specific geological unit targeted in the research.
- 20 5) **“5 Defining MPS input information”** is the most methodological section of the paper. Here, the approaches used in the comparison throughout the manuscript are described. For example, it is discussed how (and why):
 - 25 (i) **the seismic data and the existing manual adjacent model have been incorporated as hard conditioning (paragraphs “5.1 Seismic data” and “5.2 Existing 3D model”);**
 - (ii) **to translate the boreholes into soft probability to address their uncertainties (paragraph “5.3 Borehole data”);**
 - (iii) **to build an effective TI based on the outcomes of the unconstrained simulations (“5.4 Training Image”).**
- 30 6) **Section “6 Results”** is about the detailed comparisons of the outputs resulting from the application of: (i) the iterative approach for the construction of the TI and (ii) the different conditioning strategies detailed in the previous section.
- 7) **The second last section, “7 Discussion”** discusses the assumptions/choices made across the paper and their possible limitations and possible, future, developments.

8) “8 Conclusion” is a very concise section where we simply summarize our results.

We trust this is a reasonable way to present our research.

Clearly, other scientists might think differently. To some extent, it is simply matter of taste, as long as the rationale behind the choice is evident. And we believe that already in the present form, the overall logical organization of the paper is quite clear and effective. Nevertheless, in the new manuscript, we further expanded the “1 Introduction” to describe the organization of the paper.

Regarding the specific questions posed by the reviewer:

- 1) Many factors affect the quality of boreholes: (i) the drilling methods (e.g.: rotary drilling and air lift drillings); (ii) the drilling purpose (sometimes, if the goal is simply to reach a specific target, the lithological description is not a priority); (iii) the age of the boreholes (older boreholes are generally less reliable); (iv) the presence of simultaneous wireline logging data. During the geological modelling phase, all the borehole records are (or should be) checked for inconsistencies. In the study area, as stated in the manuscript, the few available deep boreholes are characterized by high level of uncertainty.
- 2) The procedure for the construction of the TI was already discussed in several parts along the original paper, however, to make our point clearer in the new manuscript, we largely expanded the section “5.4 Training image” and added three new figures (Fig.s 11, 12, and 13).
- 3) MPS has not been considered as a way to “produce 3-D subsurface information over the entire southern Denmark area more efficiently than deterministic modeling“. With the available input data (in terms of types, quality, and amount), MPS is the only way to produce a meaningful estimation of the geological variability within the Miocene at the scale that is reasonable for groundwater investigations.

As I reviewed the current draft, I assembled a list of what I consider to be its current limitations. These include:

1) Apparently, the research so far has focused on examining the role of various hard and soft conditioning data, but only a single realization is used for each setting. This is clearly insufficient. Repeated applications of MPS will produce a sequence of slightly different realizations even with the same conditioning setup, and it should be possible to quantitatively evaluate their similarities and compare this to the differences introduced by the changed conditioning strategies.

Clearly, the differences we highlighted for each conditioning setup are not realization-dependent. This means that they will appear consistently for every realization obtained with the same conditioning settings. Just to mention an example, all the realizations generated with the “borehole as hard data” (Fig. 15b, in the new version) will be “perfectly” matching all the borehole samples by construction. The same is true for the “borehole as soft data” (Fig.

15c, in the new version); in this case, we confirmed empirically that the SNESIM ignores (Hansen et al., submitted) “localized” soft data.

Of course, considering more realizations would allow uncertainty assessment. And this would be, in principle, very interesting. However, as the reviewer has pointed out, the paper is already quite long and a discussion about the uncertainty would fall out of the original scope of the manuscript. This article is, in fact, meant to be simply about the best conditioning strategy and the optimal preparation of the TI.

2) *Regarding the Training Image aspect of MPS, it seems that two TI's were used. It is unclear how they were developed and what underlying geological concepts or knowledge were used to develop them. Figure 9 does not clearly show the sand/clay layers – the colors are not ideal for this, and the text (line 15 Page 7) merely states one realization has more layers than the other. Does either seem more likely with the geological knowledge available? Are these layers defined as channels or sheets (continuous layers)? How does either TI relate to conditions within the Tønder model?*

One of the main points this manuscript would like to convey is the importance of unconditional realizations to evaluate the effectiveness of the selected TI. In particular, we discuss this in the new “5.4 Training Image” and by using three additional figures (Figs 11, 12, 13).

In addition, in the extended version of section “5.4 Training Image”, we provide further details and underline that: (i) the first TI test was based on the existing 3D geological model (the Tønder model) covering an area adjacent to the simulated one; (ii) then, during several iterations, this first TI was manually adjusted based on the unconditional outputs (however, in the paper, for simplicity, only the initial and final TIs are shown in Fig. 9 together with the associated unconstrained realizations in Fig. 10); (iii) this iterative process was stopped as soon as the corresponding realization was able to mimic the geological features expected in the Miocene.

Those expectations about the geology are based: (i) on our prior geological understanding of the area, (ii) the available seismic lines, and (iii) the few existing deep boreholes.

3) *The assessment of the results is mostly qualitative. Quantitative tools to do exist and should be used.*

With respect to a quantitative analysis of the proportions variability, we think that our point concerning the effectiveness of using the kriged sand probability to enforce the proper spatial trend is clearly demonstrated via the comparison between Fig 17b and Fig. 8. In fact, the two figures allow a voxel-by-voxel comparison between the soft conditioning distribution and the final corresponding realization. However, to meet the requests of the reviewer, we included an additional figure (Fig. 18) with the cross-correlation between the kriged sand probability (Fig. 8) and the realizations (c) and (d) in Table 1 (showed, for example, in Fig. 14c and Fig. 14d). Not surprisingly, the correlation with the realization (d) has a much more pronounced and higher maximum.

Regarding the quantitative assessment of the patterns produced by using the two different TIs in Fig. 9, in the new version, the distributions of the size, eccentricity, and jaggedness of the connected bodies in the realizations in Fig. 10 are compared in the new Figs 11, 12, and 13, respectively. Also in this case, the new figures further confirm what is
5 evident from Fig. 10a and Fig. 10b.

4) *The cited literature appears to miss several important more recent studies. Attached are a few representative paper citations.*

10 **In the revised version, we added several, relevant, references.**

FINAL COMMENTS

*MPS is an interesting and potentially powerful method for developing very useful subsurface geological models. I am aware that at least some of the authors have experimented with other simulation approaches, such as TPROGS to apparently
15 successfully simulate facies heterogeneity in buried valleys. It would be interesting for them to include at least a short comparison between MPS and other simulation approaches. The current paper assumes the reader to be proficient in MPS concepts. This may not be true in many cases, so a short comparison in the introduction might broaden the readership and understanding of the importance of this line of investigation.*

20 **We believe that the paper (already “quite lengthy in its current form”) would not benefit from a comparison with other simulation approaches as the manuscript is not about checking the performances of MPS as a tool to incorporate complex statistical information against other “simpler” approaches. This article deals solely with the optimal strategies (within the MPS framework) for the soft/hard conditioning and for the construction of the most (geologically) effective TI.**

25 **In addition, the approach of the submitted article is based on TIs for the description of the information about spatial structures, while TPROGS does not make use of TIs and, instead, requires the user to define transition probabilities from which the realizations are then simulated. Therefore, given the topic of the paper, it is not natural to consider the use of TPROGS.**

30 *I believe the ultimate goal of this research is not to model the Miocene of southern Denmark as a purely academic exercise, but to use this information to guide groundwater management schemes. I wonder what groundwater model sensitivity analysis would yield in terms of necessary subsurface detail for producing acceptable groundwater resource management at regional or site-specific scales?*

Obviously, somewhat less precise spatial definitions are likely to be required for regional assessments. On the other hand, site-specific studies may be unreliable if based only on MPS inputs without careful additional local conditioning. So, the question arises, "Where does MPS fit within this overall objective?" This question also reflects on the limitation noted on page 9 (lines 13-15) the present inability of MPA to handle graben structures and faults.

5

The present paper is about: (i) how to include, in the most effective way, the available data as simulation conditioning, and (ii) how to build a TI that is capable to reproduce the geological features we want to see in the realizations. In particular, regarding point (ii), the ability to generate meaningful geological realizations must be seen in a general perspective and, so, relevant per se.

10 Moreover, MPS is a way to "see" beyond the (strictly speaking) available data. In fact, via the prior geological knowledge formalized by the TI, it is possible to "reconstruct" features compatible, at the same time, with the data (e.g.: the geophysical measurements), but also with the desired prior geostatistical information. This is a very important aspect in the paper: a significant amount of data - but not as much as we desired (as always happens) - was available together with the knowledge of the geological features we wanted to see in the realizations. Thus, we

15 investigate the best workflow to utilize the full potential and flexibility of MPS methodology to jointly exploit those two pieces of information and obtain a realization that is, simultaneously, matching the data (i.e., boreholes, geophysical measurements, and pre-existing geo-models), and having the required spatial characteristics.

The scale of the geo-features necessary for flow modelling purposes is hard to decide before entering in the more hydrological aspects of the problem. In the paper, we show how to get those features in an effective way and we test

20 the proposed approach at the scale we think is the more appropriate one. Further analysis would be definitely necessary, but we think they are not falling in the scope of the present study.

Despite my several criticisms, I think this is a potential important paper and hope the authors will consider reorganizing it and adding in a few details on some important methodology issues, while at the same time focusing on the TI and

25 conditioning strategies.

SOME SUGGESTED REFERENCES:

- Boucher, A. (2011) *Strategies for Modeling with Multiple-point Simulation Algorithms*. IN: "Closing the Gap", 2011 Gussow Geoscience Conference, Banff, Alberta. 9p.
- 30 Kessler, T. (2012) *Hydrogeological Characterization of Low-permeability Clayey Tills – the Role of Sand Lenses*. PhD Thesis, Department of Environmental Engineering, Technical University of Denmark, Lyngby, Denmark. 80p.
- Klenner, R., Braunberger, J.R., Dotzenrod, N.W., Bosshart, N.W., Peck, W.D. & C.D. Gorecki (2014) *Training Image Characterization and Multipoint Statistical Modeling of Clastic and Carbonate Formations*. PowerPoint Presentation, 2014 Rocky Mountain Section AAPG Annual Meeting, Denver, Colorado. 27 slides.

Meerschman, E., Pirot, G., Mariethoz, G., Straubhaar, J., Van Meirvenne, M. & P. Renard (2013) A Practical Guide to Performing Multiple-Point Statistical Simulations with the Direct Sampling Algorithm. Computers & Geosciences. 52. p. 307-324.

5 *Straubhaar, J., Walgenwitz, A. & P. Renard (2013) Parallel Multiple-Point Statistics Algorithm Based on List and Tree Structures. Mathematical Geosciences. 45. p. 131-147.*

Straubhaar, J., Renard, P. & G. Mariethoz (2016) Conditioning multiple-point statistics simulations to block data. Spatial Statistics. 16. p. 53-71

Response to Reviewer #4 comments

We thank Dr. Xin He for his valuable comments and suggestions. They certainly improved the manuscript. In the following, we provide the response to the individual comments. The original review is quoted in *italics*, while our response is given in **bold** font.

5

The study aims to establish a workflow to carry out Multi-Point Statistics modeling for a testing area in Denmark using alternative 3D training images and various conditioning strategies. The research topic is of high relevance to those who work with hydrogeological modeling. The manuscript is well written with accurate language, rational methodology and convincing results. I recommend the manuscript is accepted for publication with minor revision. However, there are several

10 *details to be considered which are listed as follows:*

As stated in the abstract, the introduction and the conclusion sections, one of the most important steps of the workflow is to develop 3D TIs in an iterative way. However, this part is only briefly mentioned in the method section and not at all mentioned in the result section. I am curious about how the TIs are evolved gradually with feedback information after each

15 *step of adjustment, namely from the initial TI to the final TI.*

Additionally, is Fig 9 showing the initial or the finally TI?

We definitely see the reviewer's point and, in the new version of the manuscript, we added further details regarding the development of the TI, from the initial guess, TI1, in Fig. 9a, to the final result, TI2, in Fig. 9b. In particular, in

20 **the revised paper, we stressed the fact that: (i) the first TI simply consists in a portion of the adjacent, pre-existing, geological model (the Tønder model); (ii) then, this initial attempt has been iteratively and manually adjusted based on the output of the associated unconstrained simulation; (iii) this iterative process ended when the final unconstrained realization was found satisfactory in terms of its ability to mimic the geological features we expect in the Miocene across the study area.**

25

In the introduction section, I would suggest to add a few sentences indicating the main objectives of the study.

In the revised version of the manuscript, we followed the reviewer's suggestion.

30 *Lin 210-211. The moving window for calculating the borehole uncertainty in the vertical direction is 20 m. Meanwhile, in Fig 7(b), the thickness of the Miocene layer is about 150 m, which in principle corresponds to 7 to 8 intervals in each borehole at maximum. However, as far as I can count, there are usually more than 7 color blocks in each borehole. Am I mistaken for something?*

20 m is simply the width of the moving window. This means that the information about the categories (the lithologies) is averaged across a 20 m wide interval. This does not necessarily imply that only 7 or 8 samples remain after the application of the moving window. Actually, the size of sampling interval is unchanged, and the only minor modification on this respect consists in a loss of a certain amount of samplings at the top and bottom of the boreholes due to the fact that, in our specific implementation, we considered a window with always the same width.

Fig 7, when interpolating the borehole uncertainty, are the borehole data outside the model domain being considered, both horizontally and vertically? If not, would there be extrapolation instead of interpolation towards the edges of the model domain?

We do not interpolate the uncertainty of the borehole. Instead, we krig the sand probability of the portions of the boreholes lying within the Miocene. So, if this was the question of reviewer, generally, towards the edges of the model domain, extrapolation does occur.

In the results section, L259-266, there are two TIs being tested, one clearly has more layers than the other. Do these two TIs have any relation to the iterative approach the authors try to present in the study? Or is it a separate issue here? Moreover, it says the second TI is chosen because it is closer to what has been presented in Kristensen et al., 2015. So maybe it is better to describe very briefly what is in the Kristensen's study, and why that one is used as benchmark.

The two TIs are, respectively, the first and final test along the iterative TI development process. In particular, the second TI (TI2 - Fig. 9b) was selected to run all the subsequent conditioned simulations as the associated unconditioned realization (and not the TI2 itself) was found able to mimic the geological structures characterizing the Miocene in the study area. The characteristics we expect for the Miocene structures are described in Kristensen et al., 2015 and discussed in the manuscript in the dedicated section "4 Establishing framework-model constraints" (and in the associated Figs 2, 3, 4, 5).

Multiple-point statistical simulation for hydrogeological models: 3D training image development and conditioning strategies

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Abstract. Most studies about the application of geostatistical simulations based on multiple-point statistics (MPS) to hydrogeological modelling focus on relatively fine-scale models and concentrate on the estimation of facies-level, structural uncertainty. Much less attention is paid to the use of input data and optimal construction of training images. For instance, even though the training image should capture a set of spatial geological characteristics to guide the simulations, the majority of the research still relies on 2D or quasi-3D training images. In the present study, we demonstrate a novel strategy for 3D MPS modelling characterized by: (i) realistic 3D training images, and (ii) an effective workflow for incorporating a diverse group of geological and geophysical data sets. The study covers an area of 2 810 km² in the southern part of Denmark. MPS simulations are performed on a subset of the geological succession (the lower to middle Miocene sediments) which is characterized by relatively uniform structures and dominated by sand and clay. The simulated domain is large and each of the geostatistical realizations contains approximately 45 million voxels with size 100 m x 100 m x 5 m. Data used for the modelling include water well logs, high-resolution seismic data, and a previously published 3D geological model. We apply a series of different strategies for the simulations based on data quality, and develop a novel method to effectively create observed sand/clay spatial trends. The training image is constructed as a small 3D voxel model covering an area of 90 km². We use an iterative training image development strategy and find that even slight modifications in the training image create significant changes in simulations. Thus, the study underlines that it is important to consider both the geological environment, and the type and quality of input information in order to achieve optimal results from MPS modelling. In this study we present a possible workflow to build the training image and effectively handle different types of input information to perform large-scale geostatistical modelling.

1 Introduction

Simulation of groundwater flow and solute transport requires representative hydrogeological models of the subsurface. While many studies focus on estimating the spatial distribution of hydraulic properties (i.e. hydraulic conductivity, porosity), the reliable delineation of the underlying geological structural or hydrostratigraphic model is far more important to ensure the reliability of groundwater flow predictions (e.g. Carrera, 1993; Liu et al., 2004a; Renard and Allard, 2013).

Early geostatistical methods (e.g.: Chiles and Delfiner, 1999; Deutsch, 2002) provided tools to model uncertainty in smoothly varying Gaussian properties, like porosity or permeability within targeted rock formations (e.g., oil reservoirs). These produced petrophysical models that generally improved mineral resource development, but the models were poor when abrupt changes in rock type, and hence petrophysical properties, were important in defining reservoir structure. Later generations of geostatistical methods ~~provided~~^{supplied} tools for modelling rock types (i.e., lithology or facies), that provided incremental improvement (Stafleu et al., 2011), but still did not effectively model non-stationary patterns in rock type, and poorly captured patterns in stratigraphical units that are typically complex combinations of rock type.

Without suitable tools for developing realistic uncertainty-informed models of either non-stationary rock type or hydrostratigraphy, groundwater models are typically based on single, deterministic geological framework models that are manually constructed. Research has continued to explore methods for uncertainty-based simulation of structural heterogeneities (Huysmans and Dassargues, 2009; Kessler et al., 2013) to better estimate uncertainties in groundwater flow (Feyen and Caers, 2006; He et al., 2013; Poeter and Anderson, 2005; Refsgaard et al., 2012).

The multiple-point statistics (MPS, Guardiano and Srivastava, 1993; Strebelle, 2002) was developed with the objective to better reproduce complex geological patterns than other available geostatistical modelling techniques. The method combines the ability to condition the realizations to hard data (information without uncertainty) and soft data (information with uncertainty) with the ability to reproduce geological features characterized by statistical properties described through a so-called Training Image (TI).

Hence, the TI plays a crucial role and should be constructed to represent the structural patterns of interest (Hu and Chugunova, 2008; Maharaja, 2008; Pickel et al., 2015). However, a fundamental challenge for the use of MPS for 3D hydrogeological modelling lies in the difficulty to produce realistic 3D TIs (e.g., Pérez et al., 2014, Ronayne et al., 2008), and most of the studies in the literature are therefore based on 2D or quasi-3D TIs (Jha et al., 2014; Comunian et al., 2012; Feyen and Caers, 2006). Several researches have demonstrated the potential of the MPS to simulate 2D patterns (Hu and Chugunova, 2008; Liu et al., 2004b; Strebelle, 2002), but less attention has been given to the construction of real three-dimensional TIs.

In the present study, we describe a strategy to develop effective and realistic 3D TIs based on the a posteriori analysis of the associated unconstrained realizations.

Concerning the use of conditioning data, it is extremely important to address the fact that the data are characterized by different uncertainty levels and scales (He et al., 2014; McCarty and Curtis, 1997). In this study, available sources of

information are seismic lines, boreholes, and a pre-existing, manually constructed geo-model. Depending on their scale and uncertainty, we developed a practical way to incorporate all of them into the Single Normal Equation Simulation (SNESIM) workflow as it is implemented in SGEMS (Remy et al., 2009). The approach is general and can be readily extended to other data types.

In summary, the main objectives of the present study concern: (i) the iterative development of effective 3D TIs, and (ii) the optimal strategy for the simulation conditioning.

The paper is organized as follows: (i) section “2 Study area” deals with the overall geological framework of the area under investigation, while section “3 Data” describes the amount and characteristics of the different kinds of available data; (ii) section “4 Establishing framework-model constraints” goes into details about the specific geological unit targeted during the stochastic simulations; (iii) “5 Defining MPS input information” is the most methodological section and consists of the presentation of the different approaches whose outputs are then compared in the subsequent section “6 Results”; (iv) the second last section, “7 Discussion”, is about the assumptions/choices made across the paper and their possible limitations and future developments; (v) “8 Conclusion” is a very concise section where we simply summarize our results.

2 Study area

The study area covers 2810 km², from coast to coast in the southern part of Jutland, Denmark, and northern portion of Germany (Fig. 1). A part of this area (625 km²) has formerly undergone 3D geological modelling (the Tønder model, Fig. 1) which is presented in Jørgensen et al. (2015). In this paper, we will concentrate on the Miocene sediments within the model domain. The Miocene sediments were selected because: (i) they are primarily composed of two main hydrogeological facies: clay and sand, and (ii) the unit is composed of rather uniform structures throughout the area and therefore possible to describe in a 3D TI.

A conceptual sketch of the geology in the area is shown in Fig. 2. The base of the regional groundwater flow system corresponds with the top of the very fine-grained Paleogene clays that have a gentle dip towards the southwest. The overlying Miocene sediments consist of marine clay with sandy deltaic lobate layers. The Miocene deposits in Jutland has been thoroughly studied by Rasmussen et al. (2010) who based the studies on sedimentological and palynological investigations of outcrops and cores, combined with interpretation of high-resolution seismic data. During the Miocene, the coastline fluctuated generally northeast-southwest across Jutland, resulting in a deltaic depositional environment. Rasmussen et al. (2010) divided the Miocene deposits into three sand-rich deltaic units that are interfingered with prodeltaic clayey units. In periods with low water levels, the coastline was situated far to the southwest and coarse-grained sediments were consequently deposited in the study area. When the water level was high, the coastline was situated further to the northeast, resulting in deposition of marine clays. The delta lobes dominate in the northeast and show smooth dips towards southwest. In middle and upper Miocene, very fine-grained marine clays belonging to the Måde Group were deposited in the western part of the model domain.

The unconformable boundary between the Quaternary and the Miocene is often scoured by buried valleys (Fig. 2). The Quaternary deposits mainly consist of till and various meltwater deposits, but, in some places, also of interglacial and postglacial deposits. In some areas, the Quaternary deposits are heavily deformed due to glaciotectonism. In the western portion of the study area, the geology generally consists of outwash sandurs surrounding old pre-Weichselian moraine landscapes. The outwash sandurs show a low relief with a gentle dip towards west, whereas the old moraine landscape shows a more irregular relief up to 60 meters above sea-level (m.a.s.l). In the east, the younger morainic landscape from the Weichselian shows topographic changes between 40 - 90 m.a.s.l. The model area is influenced by a large fault-bounded structure (the Tønder graben structure, Fig. 1b) that offsets the deeper Top Chalk surface of about hundred meters (Ter-Borch, 1991). The faults clearly offset both the top of the Paleogene and the bottom of the Quaternary.

10 3 Data

3.1 Borehole data

The borehole data in the Danish portion of the study area are extracted from the Danish national borehole database, the 'Jupiter' database (<http://jupiter.geus.dk>), and comprise about 9 000 boreholes with lithological information from driller's logs and sample set descriptions. The Jupiter database provides information on a number of parameters about each borehole, which enables an evaluation of borehole data quality. ~~In the study area, many borehole records are of low quality.~~ Boreholes, like any other kinds of data, are affected by uncertainty. The level of uncertainty determines the quality/reliability of the measurements (i.e., the quality/reliability of the boreholes). Many factors impact the quality of boreholes. Just to mention a few of them: (i) the drilling methods (e.g.: rotary drilling and air lift drillings. In some cases, for example, the finer sediments can be flushed out and the driller could potentially misinterpret a clay layer as more sandy); (ii) the drilling purpose (sometimes, if the goal is to reach a specific target, the lithological description can be poor since it is not a priority); (iii) the age of the boreholes (for example, nowadays, in Denmark, samples are collected systematically every meter, and this was not the case few years ago); (iv) the presence of simultaneous wireline logging data (these kinds of ancillary information make the geological interpretation definitely more certain). During the geological modelling phase, a skilled geologist should go through all the borehole records and verify all these different pieces of information and check for inconsistencies. This is (or should be) the standard procedure to assess the quality of the boreholes and prepare the data for the subsequent geo-modelling phases. ~~In the study area, many borehole records are of low quality.~~ ~~Furthermore~~ Together with the Danish boreholes, geological information from about 500 boreholes located within the German portion of the study area and deeper than 10 m are included in the analysis. The majority of the boreholes in both the Danish and the German area are quite shallow and, in total, only 2 % of all the boreholes are deeper than 100 m (Fig. 1).

3.2 High-resolution seismic data

The seismic data are extracted from the Danish geophysical database ‘Gerda’ (Møller et al., 2009). Most of the seismic lines were conducted with the purpose to investigate the groundwater resources and examine the Miocene sediments (Rasmussen et al., 2007). In the study area, seismic lines for a total length of around 170 km (Fig. 1) were collected by several contractors with two slightly different acquisition systems that, for sake of clarity, we conventionally indicate here with SYS_COWI and SYS_RAMBØLL. In both cases, the lines were acquired as landstreamer high-resolution seismic data (Vangkilde-Pedersen et al., 2006) by using seismic vibrators as energy source. The frequency ranges spanned: from 50 Hz to 350 Hz, for SYS_COWI, and from 50 Hz to 400 Hz, for SYS_RAMBØLL; for both systems, the sweep was 5 s long. The receiver arrays consisted of: 95 not-equally spaced geophones (1.25 m between the first 32 geophones, and 2.5 m for the others), for SYS_COWI, and 102 geophones (1.25 m between the first 50 geophones, and 2.5 m for the others), for SYS_RAMBØLL. In both acquisition settings, the sources were fired every 10 m.

Under normal circumstances, the data are high quality between approximately 30 m to 800 m in depth. Prior to the import of the seismic data to the geological interpretation software, the elevation values are adjusted, based on an assumed constant seismic velocity of 1 800 m/s (Kristensen et al., 2015), which is a common velocity for Miocene and Quaternary deposits in Denmark (Høyer et al., 2011; Jørgensen et al., 2003). Elevation corrections are important because of the considerable effect of the topography that, even if mildly varying, along extended profile can significantly affect the quality of the final results.

4 Establishing framework-model constraints

The MPS model domain corresponds to the lower and middle Miocene sediments which are positioned below the Måde Group and above the Top Paleogene surface (Fig. 3). Inside the Tønder model area (Fig. 1), however, the results of the already existing model (Jørgensen et al., 2015) are used and therefore are not included in the MPS simulations. The Tønder model results are used because the model was constructed based on very thorough geological analyses and so considered as the best geological model obtainable in that area. The surfaces of the relevant geological boundaries: Top Paleogene, Bottom Måde and Top pre-Quaternary (Fig. 3) are constructed in the geo-modelling software package Geoscene3D (I-GIS, 2014) by using interpretation points and interpolating these data to create the corresponding stratigraphical surfaces. The top of the MPS model domain is obtained by merging the surfaces of the Bottom Måde and the Top pre-Quaternary surface (Figs. 3 and 4a). The lower boundary of the model domain corresponds to the Top Paleogene surface (Figs. 3 and 4b).

The top surface of the Miocene sediments shows a regional dip towards west with significant depressions along the Tønder graben structure and at the buried valleys. The surface elevation ranges from 20 m.a.s.l. to -460 m.a.s.l. (Fig. 4a), corresponding to depths varying between 30 m and 80 m, in the east, and of about 160 m, in the west. In the Tønder graben, the depth to the top of the Miocene ranges approximately from 260 m to 320 m and locally (associated with buried valleys) up to 460 m. The bottom surface of the Miocene sediments (Fig. 4b) varies more smoothly, and also has a small regional dip from east (near elevation -100 m.a.s.l.) to west (approximately elevation -320 m.a.s.l.), punctuated primarily by the Tønder

graben structure (elevation down to -560 m.a.s.l.). The Miocene sediments typically have a thickness varying between 50 m and 250 m, but are thinner and locally absent below the buried valleys (Fig. 2).

5 Defining MPS input information

5.1 Seismic data

5 Rasmussen et al. (2010) proposed a lithostratigraphy for the Miocene succession, a “Miocene model” (Kristensen et al., 2015), based on interpretations of seismic data that was correlated with borehole interpretations and outcrops. The observational data points used in the Miocene model were utilized in our study to define the top of individual Miocene stratigraphical formations along the seismic lines (Fig. 5a). In order to use this information in the MPS modelling, the stratigraphical interpretations from the Miocene model are translated into a binary sand/clay voxel model of one cell width
10 along each seismic line (Fig. 5b and 6).

The sand/clay distribution along the seismic lines is used as hard data in the MPS simulations. The information is used as hard conditioning since it is considered highly reliable, and since the scale of structures delineated by the seismics is comparable to the scale of the simulated output.

5.2 Existing 3D model

15 | In order to ensure edge matching between the stochastic realizations and the deterministically ~~modelled-constructed~~ Tønder model, a buffer zone along the pre-existing model’s edges is created within GeoScene3D and used as hard conditioning data for the MPS simulations. The Miocene formations interpreted in the existing Tønder model (Jørgensen et al., 2015) are translated into sand and clay. In ~~Figure-Fig.~~ 6, the hard conditioning data from the pre-existing model (the buffer zone) are shown together with the hard information from the seismic lines.

20 5.3 Borehole data

All lithological categories contained in Jupiter are simplified and divided into three groups: sand, clay and ‘other’. In this study, the conditioning based on the boreholes has been conducted through the use of three different strategies. The different ways of considering the borehole information are illustrated and summarized in Fig. 7.

The simplest and most common approach for exploiting the information from the boreholes is to include them as hard
25 conditioning data. This is the first test performed in the present study (Fig. 7a). However, this simple approach does not take into consideration the uncertainty in borehole data associated with: (i) inaccuracies in the recorded information, and (ii) the resolution, or scale, differences between the information in the borehole records and the geological model cell size.

In order to address these issues, an alternative conditioning strategy is tested. In this case, the boreholes are considered as
30 soft data (Fig. 7b): ~~In this case,~~ a 20-meter-long moving window is applied to each original borehole in order to average the

densely sampled lithological data into probabilities defined on the coarser simulation grid. Since the typical vertical dimensions of the structures are ~20 m, the size of the averaging window is chosen accordingly. This procedure is consistent with the reasonable assumption that, in the middle of the geological formation, we are relatively certain of the lithology, while this certainty decreases as we get closer to the boundaries. Moreover, in order to take the general uncertainty in the borehole information into account, we map the resulting averaged values into a sand probability interval ranging from 80 to 20 %. In this way, voxels with the highest chances of having sand are characterized by a maximum sand probability value of 80 % (in pink, Fig. 7b), whereas voxels with the lowest sand probability are associated to a value as low as 20 % (in green, Fig. 7b). In Fig. 7b, it is clear that the transition zones between sand and clay correspond to a band with sand probabilities of 40 %. This value is the marginal distribution value for sand occurrence within the investigated model volume, as it is calculated from the borehole data and consistently formalized in the TIs.

When borehole information is too distant, the sand/clay ratios in the stochastic realization are solely derived from the TI and the sand marginal distribution. Unfortunately, borehole information at the relevant depths is relatively sparse (due to shallow boreholes), and, at the same time, the SNESIM algorithm has a tendency to ignore such “localized” soft data (Hansen et al., submitted). Moreover, it is known that the model domain shows a slight spatial lithological variation in which the overall proportion of sand is higher in the northeast compared to the southwest (that is also clear from the borehole data). To enforce this real, general trend in the realisations, the “localized” borehole probabilities are kriged into a 3D grid to be used as “diffuse” soft conditioning (Fig. 7c and Fig. 8). This would be unnecessary if SNESIM could handle soft data as local conditional probability and, here, we are suggesting a practical strategy to effectively overcome this limitation. Clearly, the kriged sand probability distribution is seen to correspond to the boreholes close to their locations (Fig. 7c), whereas areas far from boreholes (e.g., at km 6 along the section in Fig. 7c) appear white (so characterized by a sand probability equal to 40 %). However, in a few cases (e.g. the clay layer in the deep part of the borehole at profile distance 10 km, Fig. 7c), the borehole information does not seem to migrate into the surrounding grid. This can be explained by the influence of other boreholes in the 3D domain. The desired spatial trend, characterized by a higher sand probability in the north-east compared to the south-west, is evident in the sand probability grid (Fig. 8).

5.4 Training image

The training images (TIs) are constructed as 3D voxel models with the same discretisation as the entire model (100 m by 100 m laterally, and 5 m vertically) and consist in approximately 500 000 voxels, covering an area of 90 km². The sizes of the TIs are significantly smaller than the simulation domain, but they are large enough to cover the size of the typical structures in the simulated Miocene unit. The TIs are used by the MPS simulation algorithm to represent the basic spatial and proportion relationships of the sand and clay facies within the Miocene unit. Hence, the TIs are modelled to show deltaic sand layers building out towards southwest within a larger clayey unit. The sand content in the TIs is 40 %, in accordance with the proportion of sand observed in the borehole data.

The TIs are built in Geoscene3D using the voxel modelling tools described in Jørgensen et al. (2013). In practice, each sand and clay layer is defined by so called “-interpretation” points. These points are subsequently interpolated into surface grids, which are used to delineate defining the volumes, which subsequently are then populated with sand and clay voxels. Thus, by manually changing the locations of these interpretation points and/or creating/deleting some of them, we can have a full control over the adjustments of the TIs.

In the present study, several different TIs were tested, and, for sake of simplicity, only two of them (the first attempt and the final TI) are explicitly showed in this paper (Fig. 9). The first TI (TI1 - Fig. 9a) is based on the existing 3D geological model covering an adjacent area (the Tønder model; Jørgensen et al., 2015). The first TI has been manually adjusted, during several iterations, based on the unconditional outputs. This iterative process stopped when the corresponding unconstrained realization was found satisfactory in terms of its ability to mimic the geological features we expect in the Miocene across the study area. Those expectations about the geology are based on our prior geological understanding of the area, the available seismic lines, and the few existing deep boreholes. For example, the unconditioned realizations, associated with the TIs in Fig. 9, are shown in Fig. 10. The main difference is that TI1 has more layers than the second one (TI2 - Fig. 9b). This is clearly reflected in the unconditioned simulations, in which, the realization based on TI1 (Fig. 10a) shows significantly more layers than the corresponding realization based on TI2 (Fig. 10b). The results are evaluated and compared against the structures expected from the Miocene model (Kristensen et al., 2015). Hence, to adhere to what we know about the Miocene geology, the unconstrained realization associated with the selected TI was supposed to show fewer, larger, and more compact sand structures. These characteristics are evident if we directly compare the two realizations in Fig. 10, and clearly confirmed by the study of the associated distributions in Figs 11, 12, 13 (see, for instance, Haralick and Shapiro, 1992). In particular, Fig. 11 quantitatively demonstrates that larger sand bodies are more frequent in the realization corresponding to TI2 (black histogram), while the realization generated by TI1 (green histogram) is characterized by a significantly higher presence of relatively small sand layers. Regarding the shape of the features of the realizations in Fig. 10, Fig. 12 highlights that elongated sand structures are more probable for the realization in Fig. 10a (in fact, eccentricity equal 1 corresponds to the degenerate case of a straight line). Jaggedness, defined as the ratio between the surface and the size of bodies, can provide a useful estimation of the compactness of the sand bodies (Fig. 13). Not surprisingly, the sand lenses in the realization associated to TI1 are more jagged than those in the other realization obtained by using TI2. Because of the higher accordance between our geological expectation of the Miocene in the area and the unconstrained realization in Fig. 10b, TI2 is selected for all MPS simulations discussed in the rest of the paper.

6 Results

In this study, two different TIs are tested (Fig. 9). The associated unconditioned realizations are shown in Fig. 10. Both TIs represent a primarily clayey sequence, interrupted by sand layers showing a smooth dip towards southwest. In both TIs, the sand content amounts to approximately 40 %, which is the total sand content of the entire Miocene unit calculated from borehole data. The main difference is that the first TI (Fig. 9a) has more layers than the second one (Fig. 9b). This is clearly

~~reflected in the unconditioned simulations in which the realization based on the first TI (Fig. 10a) shows significantly more layers than the corresponding realization based on the second TI (Fig. 10b). The results are evaluated and compared against the structures expected from the Miocene model (Kristensen et al., 2015). Consequently, the second TI is selected for all MPS simulations.~~

5 In the following, we present and compare the structures of the single realizations generated by each of the different conditional strategies analysed in this study (Table 1). All the realizations are produced by using the same random seed to better appreciate the differences. For comparison, an unconditioned realization (a) is presented in the first panel of each of the figures (Figs. ~~10-14~~ - ~~1216~~). The second panel (b) shows a realization generated by using exclusively hard conditioning. In the third panel (c) a realization is presented, in which the borehole information is directly treated as soft conditioning data. 10 Finally, in the fourth panel (d), a realization with the sand probability borehole grid used for soft conditioning is shown.

Figure ~~11-14~~ shows a horizontal slice through a realization representing each of the four conditional strategies listed in Table 1. As expected, the overall size and form of the structures are comparable between the realizations in (a)–(d) since the spatial characteristics of the structures are primarily determined by the TI. In (b), (c) and (d), the realizations within the Tønder buffer zone (delimited by the dash lines, ~~Fig. 11~~Fig. 14) are completely defined by the hard data. It can be observed 15 that the buffer zone cannot be identified in the realizations, which further supports our final choice for the TI₂. In fact, this indicates that the same kind of spatial variability and geological patterns are seamlessly present within the pre-existing Tønder model and the simulation results. In this horizontal slice, it is possible to appreciate the effect of the soft probability grid (~~Fig. 11~~Fig. 14d) compared to the case of “localized” borehole information (~~Fig. 11~~Fig. 14b and ~~11e~~14c): when using the probability grid, there is a significantly higher sand content and more interconnected sand body occurrence in the middle 20 part of the study area (compare with Fig. 8).

Figure ~~12-15~~ shows vertical profiles through each of the tested realizations (Table 1) along a transect with several deep boreholes (for location, see ~~Fig. 11~~Fig. 14). Like in ~~Fig. 11~~Fig. 14, the overall structural patterns of the individual realizations appear similar. The outcome of the unconditioned realization does not agree with the borehole information, since this has not been used. For instance, this is confirmed by the borehole at profile distance 10 km in Fig. ~~12a~~15a. On the 25 contrary, in the realization where the borehole information is considered as hard data (Fig. ~~12b~~15b), almost perfect consistency is observed between the realization and the boreholes. However, mismatches naturally occur when the individual layers in the boreholes are thinner than the simulated voxel thicknesses (e.g., by the borehole at profile distance of about 15.5 km). Another seeming mismatch in Fig. ~~12b-15b~~ occurs every time the influence of the borehole information is extremely local, sometimes limited to a single voxel corresponding to the one actually holding the borehole information. This is, for 30 instance, seen for the borehole at profile distance of about 9 km, where the fit between the realization and the deeper part of the borehole only appears when observed at a very detailed scale.

Also in the realization where the borehole information is considered as soft data (Fig. ~~12e~~15c), there is a generally good fit between the realization and the borehole data, but this match is clearly less pronounced in areas where a high uncertainty is

associated with the borehole data (Fig. 7b). For instance, a poorer fit compared to Fig. 152b is observed at profile distance of about 10 km. Generally, the fit to the boreholes is better when the soft conditioning information does not conflict with other statistical properties as defined by the TI or neighbouring conditioning information. An example of this conflict can be observed by the borehole at about 9 km. Here, the test with the hard data (Fig. 42b15b) resulted in a highly local match concentrated in a single voxel column, implying that the borehole information did not comply with neighbouring data or statistical parameters. For the same reason, the realization does not strictly fit the borehole when the borehole information is treated as soft conditioning data (Fig. 42e15c). The difference between (c), where the boreholes are treated as soft probability data, and (d), where the soft probability 3D grid is used (Fig. 7c), is most pronounced when considering the realization results on a larger scale than the shown in the profile in Fig. 4215.

A further example highlighting the effects of the probability grid is shown in Fig. 13Fig. 16, where a long SW-NE profile through each of the tested realizations (Table 1) is inspected (for location, see Fig. 14Fig. 14). Borehole data are located further away than the voxel size (100 m) and is therefore not shown on the profile. Again, the overall structural pattern is comparable between the different realizations. As also observed in the horizontal view (Fig. 14Fig. 14), and as it must be, the results in (b), (c) and (d) are fixed within the buffer zone around the Tønder model, where the hard conditioning information is used. For exactly the same reason, the realizations in (b), (c) and (d) perfectly match also where the profile crosses the seismic lines. Since the differences in the constraining strategy are related to the way the borehole data are handled, only little structural dissimilarities are seen when considering this specific profile with no borehole data. Those differences are therefore mainly controlled by the trend imposed by the soft probability grid in (d). Hence, the most pronounced difference is the higher clay content in the south-western part of (d) compared to the northeast. This spatial variation in the clay content from the west to the east is even clearer in the 3D view of the realization shown in Fig. 14Fig. 17. The kriged sand probability is effective in enforcing the proper spatial trend on the realization. This is evident, not only from the comparison between Fig. 17b and Fig. 8, which allows verifying, voxel-by-voxel, the accordance between the soft conditioning distribution and the final corresponding realization, but also from the results in Fig. 18. In fact, Fig. 18 shows the cross-correlations (see, for instance, Stoica and Moses, 2005) between the soft probability distribution (Fig. 8) and each of the realizations visible, respectively, e.g., in Fig. 14c and Fig. 14d (see, also, Table 1, cases (c) and (d)). As expected, the correlation with the realization (d) has a much higher and more pronounced maximum. It is probably important to stress that our conclusions are general as all the differences highlighted for each conditioning setup are not realization-dependent. This means that they would appear consistently for every realization obtained with the same conditioning setting.

7 Discussion

If MPS modelling is applied to large study areas, it is typically necessary to divide the area into different regions or domains and use different TIs to properly describe the geology in each individual region. In the present study, the entire investigated

area was divided into four main, vertically subdivided, units: the Quaternary, the Måde Group, the Miocene and the Paleogene. The Miocene sequence was chosen for our study since it is relatively stationary from a statistic point of view and can be easily divided into two main facies: sand and clay.

One of the challenges was the presence of the significant graben structure, which offsets the Miocene layers. In the current study, the graben structure is only visible through the morphological shape of the top and bottom of the model domain, but in the MPS realizations this has been ignored. In future studies, faults should be handled, such that the MPS simulation results are affected across the faults. A possible solution could be to use the geochron formalism (Mallet, 2004), in which the simulation could be performed in a regular grid, with geo-time as y-axis. Realizations should then be converted into depth using a geo-time to depth conversion.

The generation of 3D TIs that produce desired patterns is time consuming and difficult, which may be why many of the previous studies are based on 2D or quasi-3D TIs (Comunian et al., 2012; Cordua et al., 2016; Feyen and Caers, 2006; Strebelle, 2002). In this study, the 3D TI was created in the modelling software GeoScene3D. Since GeoScene3D is specifically designed for 3D geological modelling and hosts tools for manual voxel modelling (Jørgensen et al., 2013), the creation of the TI was relatively easy and straightforward. When creating the TI in this manner, the main focus was to represent the expected geological structures and not to make it stationary. In theory, MPS implementations assume stationary TIs (Liu et al., 2004b) and MPS application to strongly non-stationary systems is currently an area of research (e.g. Honarkhah and Caers, 2012; [Straubhaar et al., 2011](#); ~~de~~ Vries et al., 2009; [Cuhgunova et al. 2008](#)). The TI used for this study was generated by following the unique criterion that the unconditioned simulation (obtained by using SNESIM through its implementation in SGEMS) could satisfactorily reproduce the expected geological structures. Ideally, the TI should be constructed independently from the choice of MPS algorithm, and the realizations obtained by using a specific TI should have the same spatial variability as formalized by the training image. In practice though, this is rarely the case. While a specific part of the spatial statistics may be accurately reproduced, the realizations may lack geological features that can be crucial for subsequent modelling and interpretation. This is why the choice of MPS algorithm, and the parameters used to run the MPS algorithm have significant impact on the spatial structures seen on generated realizations. Hence, in practice, structural modelling should consist of choosing a TI together with a specific MPS algorithm (and the associated modelling parameters) to generate realizations capable to reflect the spatial variability that appears to be realistic from a geological perspective (Liu, 2006). Thus, the development of an effective TI involves an iterative procedure, where the realizations should be tested and evaluated. It is worth noting that even if the developed TI is not stationary, it is interpreted as stationary by the algorithm we have used (SNESIM; Strebelle, 2000). The realizations showed a significant sensitivity to the actual choice of the 3D TI (Fig. 10). Thus, we highly recommend a careful evaluation of the unconditioned simulation results and subsequent, consistent TI optimisation.

A strategy to include available information into the stochastic simulation is via hard conditioning. Through hard conditioning, the realizations are forced to perfectly match the provided data. In this study, hard conditioning was used to ensure a perfect correspondence between the simulation results and a former geological model available for the Tønder area.

The results illustrate that this goal can be successfully reached even though the influence of the hard conditioning data remains quite local.

Also the seismic data, represented by interpretations along the seismic lines, have been treated as hard conditioning data. This can be debated since seismics is an “indirect” geophysical method that is inherently affected by uncertainty. The reflections observed on seismic data represent changes in seismic velocity and/or density, but they are not necessarily related to lithological variations. Furthermore, the quality of the data can be highly varying as the resolution capability depends on the depth and, due to the uncertainty of seismic velocities used for depth conversion, also depths in the seismic sections are uncertain. In the present case, it was decided to use the interpretations along the seismics as hard conditioning data as their level of uncertainty is assumed to be much lower than the other available data (Kristensen et al., 2015), especially at the scale required for the simulation.

Because of technical and economic limitations, the application of reflection seismics for shallow hydrostatgraphic studies is relatively recent (probably the first examples can be traced back to the ‘80s). However, as a consequence of the increasing and general awareness concerning the use and protection of water resources, during the last 40 years, seismics - together with several other geophysical techniques (e.g., the airborne electromagnetic methodologies) - has been applied to many, diverse hydrogeological characterizations with varying results (e.g., Francese et al. 2005; Giustiniani et al, 2008). Several of the problems in this kind of surveys lie: (i) in the presence of anthropic noise; (ii) the fact that a possible shallow water table may reflect the majority of the energy and, at the same time, mask low velocity geological features, preventing the effective reconstruction of deeper structures. Actually, in the attempt to overcome these difficulties, it has become more and more common to process and invert what is still often considered noise: the ground-roll (Strobbia, 2009). In fact, ground-roll contains valuable information about the shear velocity distribution in the subsurface and is generally characterized by high-amplitude. Recently high-resolution, shallow techniques based on surface waves have been developed and tested successfully for hydrogeological investigations (Vignoli et al., 2012; Vignoli et al., 2016). A possible limitation of techniques based on surface waves concerns the availability of low frequency sources: in presence of slow sediments, low frequencies are required to reach the desired depths, but generating them is very demanding and potentially detrimental to the seismic vibrator.

In the present research, the use of the borehole data as hard conditioning data was considered suboptimal due to the low quality of many of the wells and the different discretization of the borehole data (1 m) compared to the size of the realization grid (5 m). The borehole data were therefore translated into soft probabilities by using a moving window strategy that, in one shot, takes into account the borehole information uncertainty and the different scale issue. A uniform uncertainty of 20 % has been assumed for the boreholes across the entire domain; however, in future studies, it would be straightforward to extend the present approach and locally rescale the soft probabilities according to a quality rate of each individual borehole as, e.g., the one presented in He et al. (2014). In this way, poor quality borehole would influence the simulation less than more reliable data.

One of the difficulties in the development of a proper MPS realization of the Miocene sequence was that the sand content varied spatially across the model domain making the sequence non-stationary. A 3D sand probability grid (Fig. 8) was generated in order to migrate the information further from the boreholes and constrain the geostatistical simulation to follow the spatial sand/clay trend characterizing the study area. The soft probability grid can consequently be seen as a shortcut to address the non-stationarity, such that the sand/clay content derived from the TI was overruled by the probability grid. Another possible solution could consist in the creation of different TIs to represent the end-members, and then interpolate these to obtain gradual changes dependent on the positions as discussed in Mariethoz and Caers (2014). Actually, if SNESIM could correctly handle soft data in the form of localized conditional probability, kriging the borehole probabilities would be unnecessary (Hansen et al., submitted).

In addition to the data already incorporated as (soft and hard) conditioning data in this study, dense electromagnetic (EM) surveys, on approximately half of the area, are available in the Danish geophysical database Gerda (Møller et al., 2009). An option would be to use these resistivity data in the MPS modelling as soft conditioning data, such that high electric resistivities indicate sand, while clay corresponds to low resistivity values (see, for instance, He et al., 2014; He et al. 2016). However, EM data have a limited resolution capability towards thin layers, especially in the deeper parts of the investigated sequences. The modelled unit is generally present at great depths (from a range between 30 m and 80 m, in the east, to a range between 150 m and 170 m, in the west) and the resolution of the EM data is consequently quite low in most of the area. This is especially the case in the west, where the Miocene unit is located below the depth of investigation (Christiansen and Auken, 2012). Another challenge regarding the use of resistivity data for detecting sand and clay within the Miocene deposits is the common occurrence of silt (Rasmussen et al., 2010). Some of the clayey formations are very silty and, while silt has small grain sizes and hydraulic conductivities, it has high resistivities. Thus, clayey formations with high silt contents might show higher resistivities than expected, leading to potentially wrong interpretations. In addition to that, during the borehole description phase, silt is often recognised as clay, and this clearly causes a mismatch between the borehole and resistivity information.

Geostatistical simulation methods are most commonly used to create multiple realizations whose variability represents the combined (uncertain) information; for instance, with the purpose to estimate uncertainties of structural variability (Feyen and Caers, 2006; He et al., 2013; Poeter and Anderson, 2005; Refsgaard et al., 2012) or to make probability calculations to be used for various forecasts (Stafleu et al., 2011, Christensen et al., 2017). In this study, only one ~~representative~~ realization of each of the conditional strategies was presented. The reason is two-fold. Firstly, the primary goal of this paper is to describe a workflow for choosing a training image, and to combine all available information into one consistent probabilistic model. And each individual realization (e.g., in Fig. 17) is, by construction, compatible with all simulation inputs (thus, the statistics from the TI, the hard data, and the soft conditioning). Secondly, the realization generated in the final test (Fig. 14 Fig. 17) was, at the end, incorporated in an overall geological model (Meyer et al., 2016): whereas, in this case, using a single realization is considered acceptable in this case since the objective is to study large-scale groundwater flow and saltwater intrusion, the use of multiple realizations for the propagation of uncertainty into, for example, hydrological models would be

~~outside the scope.~~ Thus, ~~to~~ make groundwater predictions on a large scale, the overall distribution and connectivity of the overall structures are crucial, ~~whereas while~~ the precise location of the individual structures is less important. In contrast ~~to this~~, detailed studies, like catchment analyses, would not make sense based on a single realization (He et al., 2013) ~~and - Ideally~~, assessments based on a significant number of different realizations should be conducted to investigate the variability of the outcome. ~~In practice, methods to better make use of these probabilistic models need to be developed and refined in order to utilize the multiple realizations and the uncertainty they represent.~~

The validity of the presented workflow is demonstrated for the Miocene unit characterized by relative simplicity and presence of only two categories. This does not mean that the applicability of this approach should be limited to simple situations. This research can be considered a proof of concept and its intent is to clearly show the relevance and effectiveness of our strategy in addressing the difficulties frequently encountered, even in simple cases. We do not see any particular difficulty in extending the proposed strategy to more complex settings characterized, for example, by a larger number of categories. In fact, if this is the case, dealing with three or more categories makes the preparation of the hard conditioning data (e.g., the interpretations of seismic lines) clearly more laborious, but conceptually not more difficult. The same is true for the way we handle the borehole as soft conditioning data: definitely, the implementation of the sliding window and the following kriging procedure are not different if a larger number of categories are involved. Finally, MPS approaches (together with the associated TIs) are already routinely used in situations with more than two categories (e.g., Jones et al. 2013), and, in our approach, special emphasis is placed uniquely on the strategy for the development of effective TIs via careful analyses of the unconstrained realizations.

8 Conclusions

This study investigates strategies for MPS simulations in large 3D model domains consistent with different types of input data. The strategies were tested within an area of 2 810 km² in which the Miocene unit was modelled using MPS simulation. This part of the model was chosen since the Miocene can be effectively subdivided into ~~two-few~~ categories (*i.e.*: sand and clay) and is relatively stationary in the investigated area. An already existing and detailed geological model (the Tønder model) was present in a part of the study area, and ~~this~~ was used in the final comprehensive geological model. A 3D TI was constructed based on the well-known geology of the unit. The stochastic simulations were conducted using the SNESIM algorithm as it is implemented in SGeMS. The final TI was developed iteratively by checking the outcomes of the corresponding unconditioned simulations, and adjusting it in order to obtain the most geologically meaningful structures in the final realizations. The previously published Tønder model and reliable seismic interpretations were used as hard conditioning data in order to preserve the associated information during the simulation. On the other hand, the boreholes were incorporated into the simulation workflow through different conditioning strategies. The first approach - the most traditional one - consisted of using the boreholes as hard conditioning data. This quite standard approach was not satisfactory as borehole data can have a high degree of uncertainty. Hence, via a moving window strategy, the lithological information in

the borehole was translated into a probability distribution that could address uncertainties in borehole data both from inaccuracies and scale mismatch. Unfortunately, SNESIM limits the influence of soft conditioning data to local neighbourhoods around each data value and is unable to effectively regionalize any trends that might be captured. To better address this problem, we found it straightforward and effective to use it as soft conditioning variable and kriged the sand probability derived from the boreholes into a 3D voxel model. By using this last approach, we managed to successfully reproduce the sand/clay trend across the simulation domain evaluated based on a visual inspection. The study shows a possible-practical workflow to properly build TI and effectively handle input information to be successfully used for large-scale geostatistical modelling.

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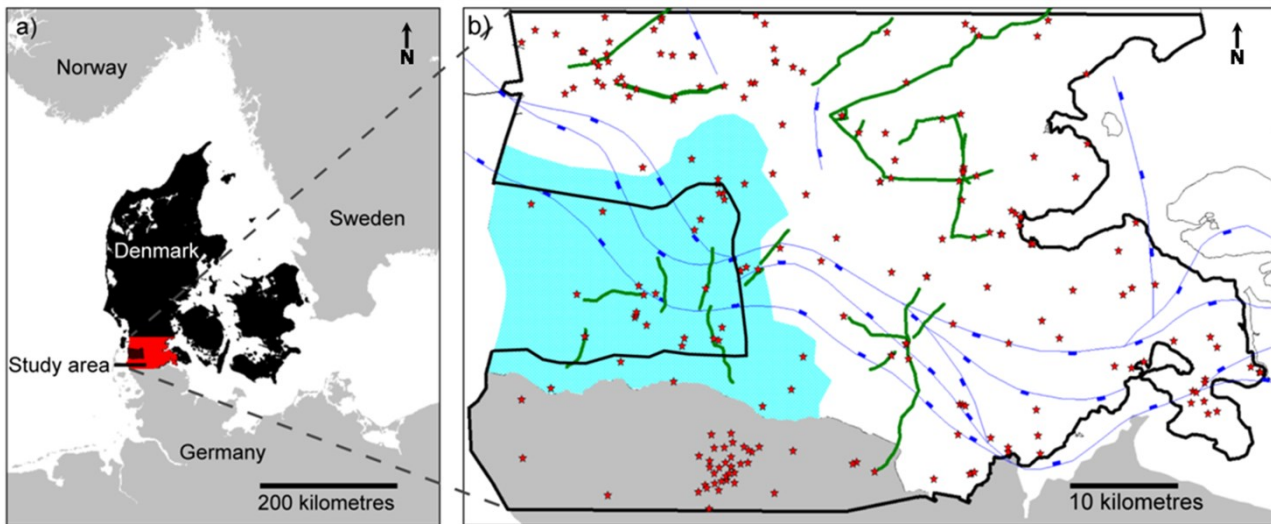


Figure 1: a) Location of the study area, b) Map of the model area (the solid black line) shown together with the data and the fault structures delimiting the Tønder graben: red stars indicate boreholes deeper than 100 m, green lines the position of the seismic lines; the Tønder graben structure is marked in blue (Ter-Borch, 1991). The turquoise shading marks the model area of the Tønder model (Jørgensen et al., 2015); the grey zone in map (b) represents Germany.

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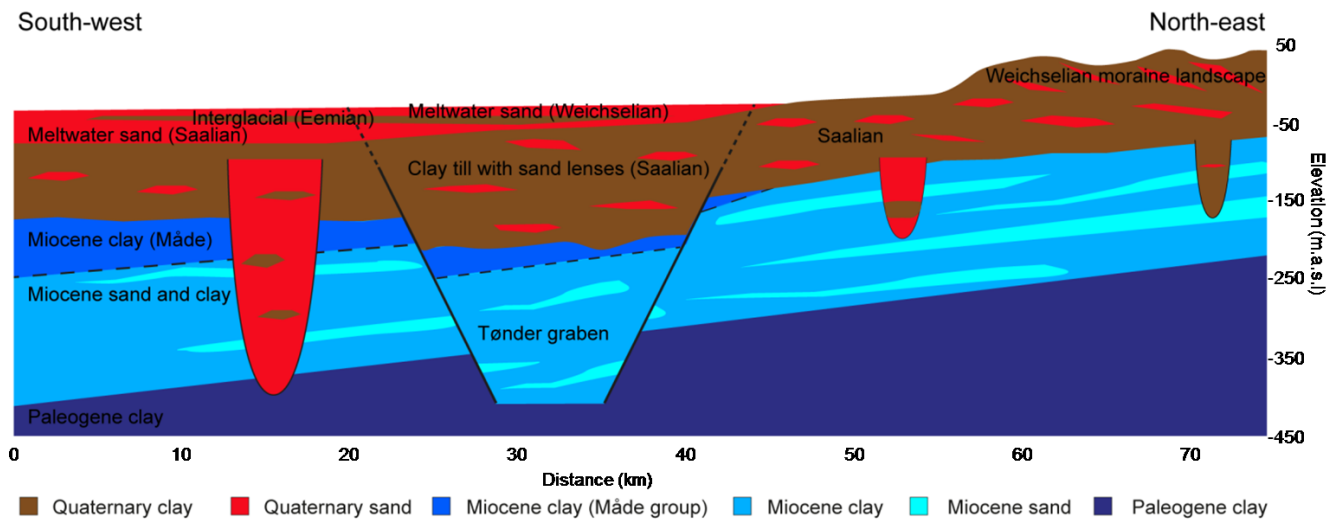


Figure 2: Conceptual sketch of the geology in the study area.

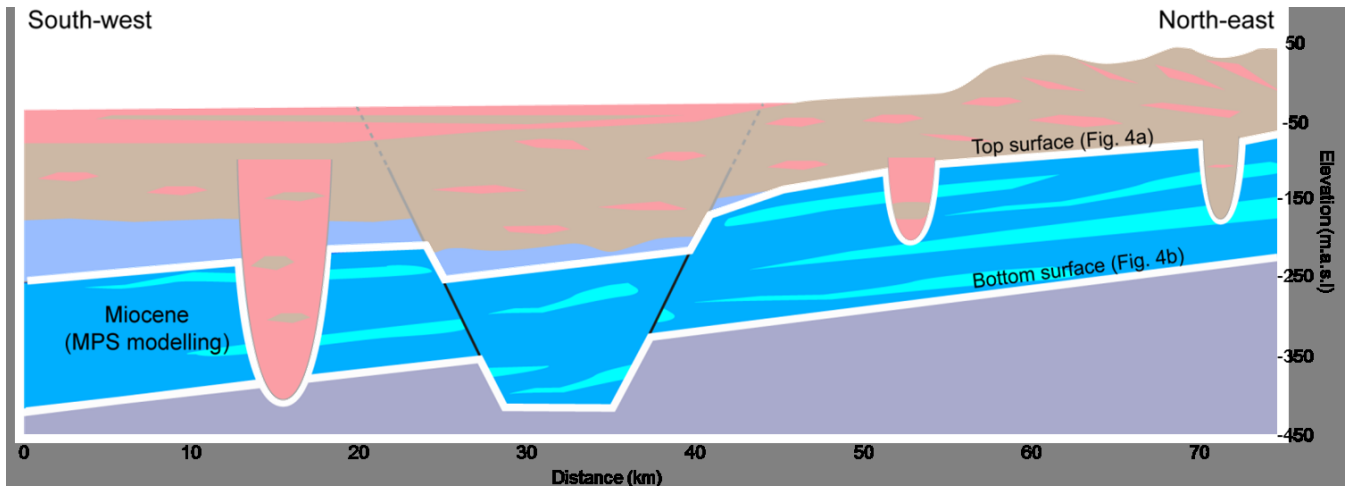


Figure 3: Sketch of the MPS model domain based on the conceptual sketch of the geology in Fig. 2: Top and Bottom of the Miocene unit is outlined by thick white lines. The surfaces are shown in Fig. 4a and 4b.

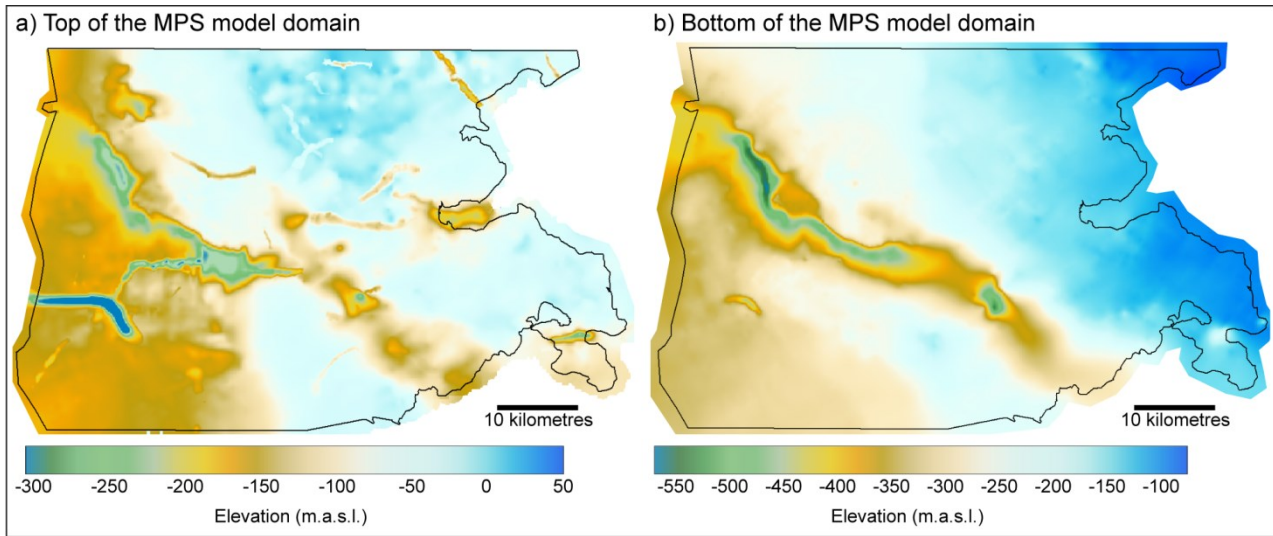


Figure 4: Elevation of the top and bottom of the MPS model domain (the Miocene unit). a) The modelled surface defining the top of the MPS model domain. The surface is obtained by merging the bottom of the Mâde Group and the top pre-Quaternary (see Fig. 3). b) The modelled surface of the bottom of the MPS model domain, which consists of the Top Paleogene clay. Note: Different colour scales.

South west

North east

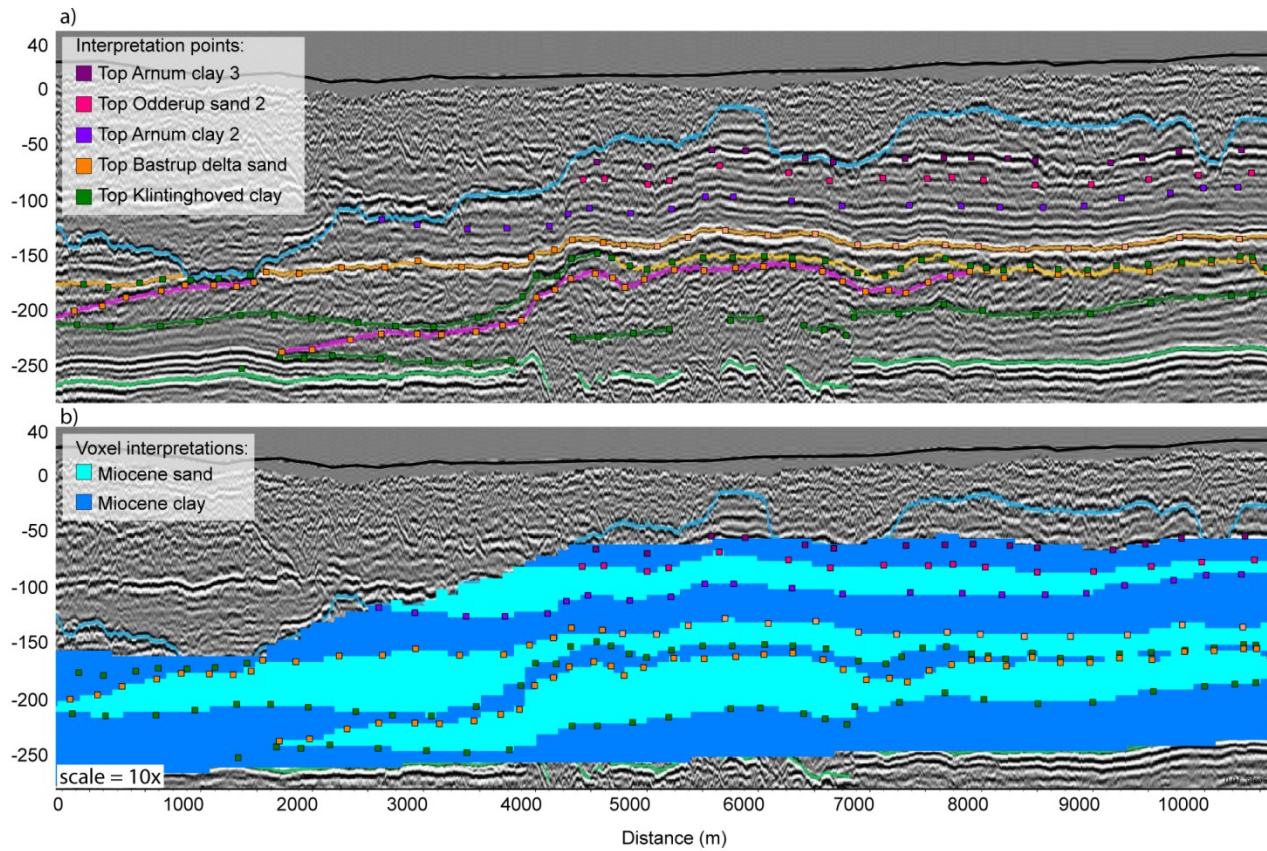


Figure 5: Preparation of seismic data input exemplified by a selected seismic section (for position, see Fig. 6). a) The seismic section shown together with coloured horizons and interpretation points derived from the Miocene model (Kristensen et al., 2015). b) The seismic section shown together with the generated “2D voxel model”. Vertical exaggeration = 10x.

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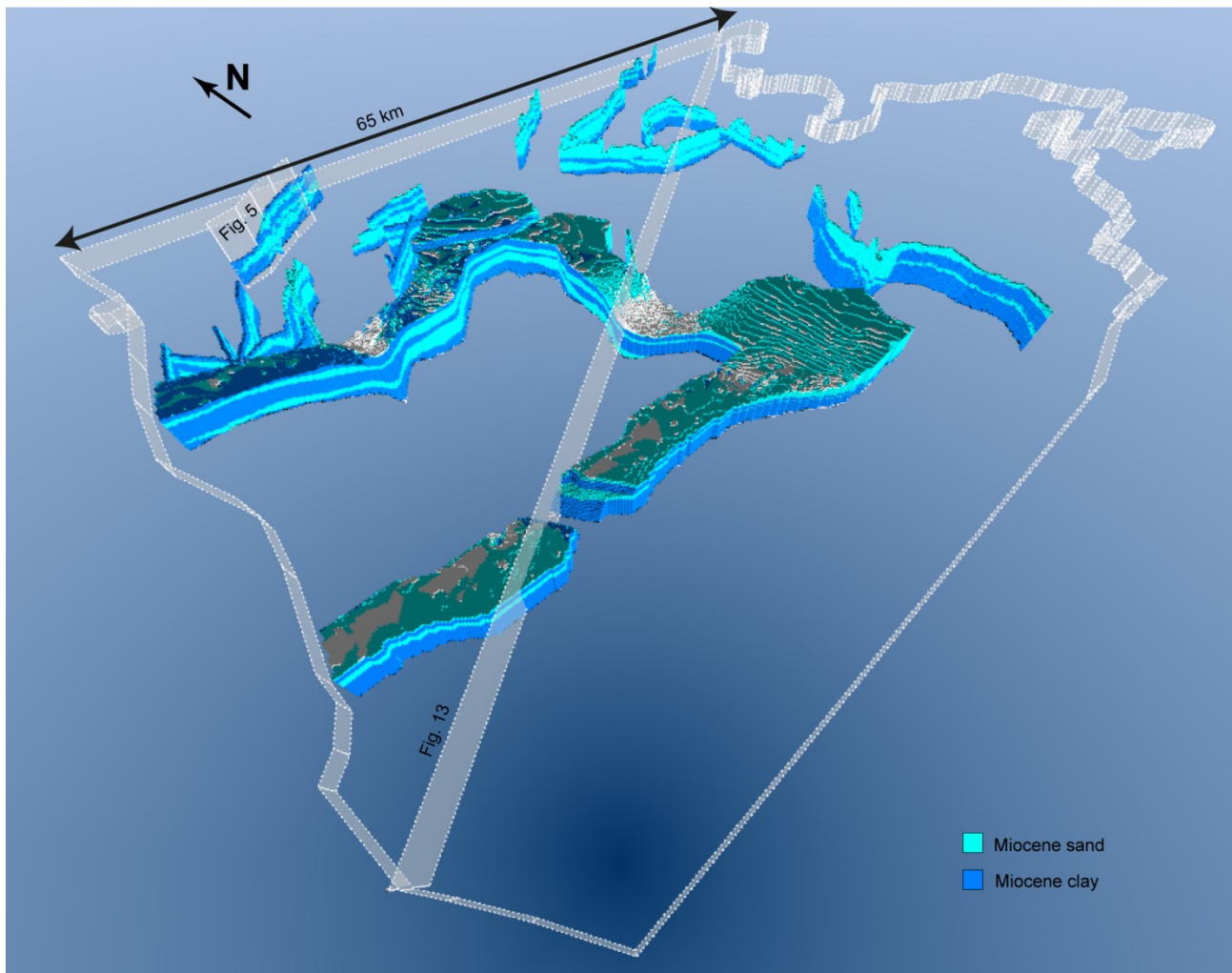
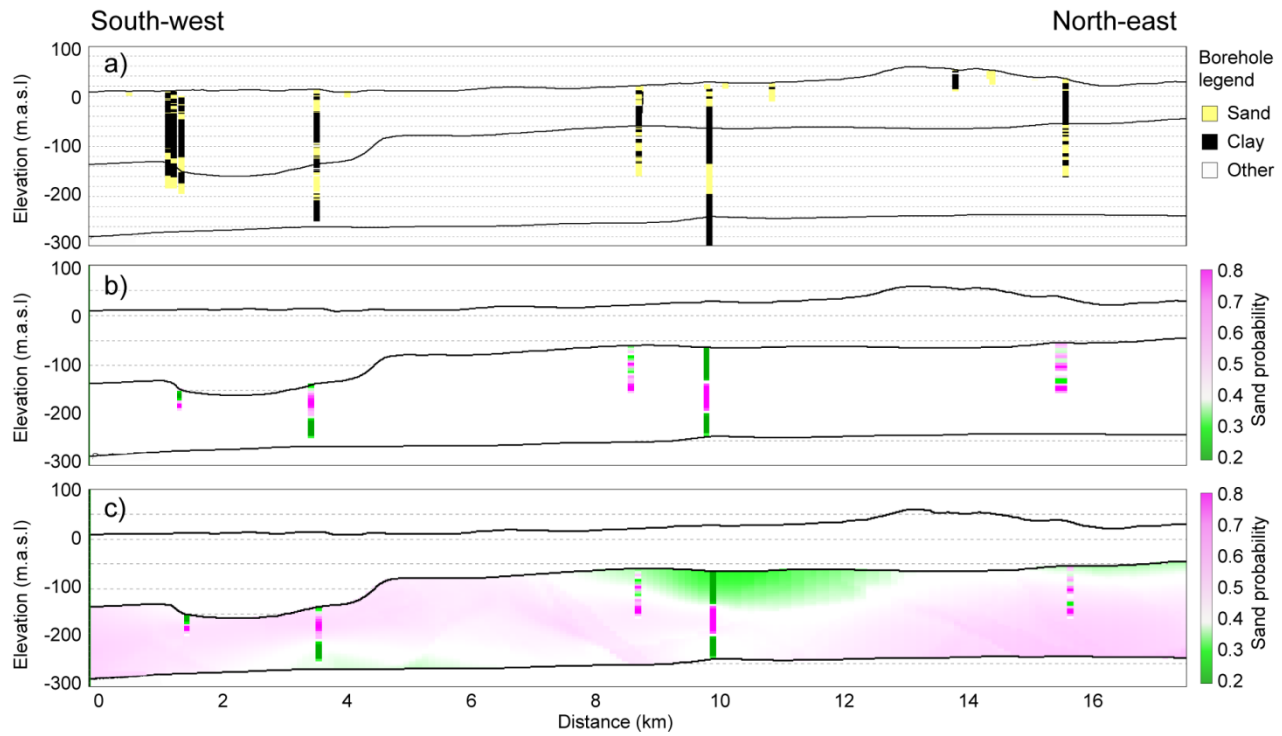


Figure 6: 3D view of the hard conditioning data (the buffer zone around the Tønder model and the seismic lines), seen from south-west. Positions of the seismic line in Fig. 5 and the profile in [Fig. 13](#) [Fig. 16](#) are marked on the figure. Vertical exaggeration = 10x.



5 **Figure 7: Three different ways to handle borehole information illustrated along a profile in the study area (for position, see Fig. 14). The resulting realizations are shown in Fig. 12. a) The sand/clay occurrence in the borehole is considered as hard data. b) The sand/clay occurrence is translated into sand/clay probability and then considered as soft data. c) The sand probabilities from the boreholes are kriged into a 3D grid to be used as soft conditioning. Vertical exaggeration 8x.**

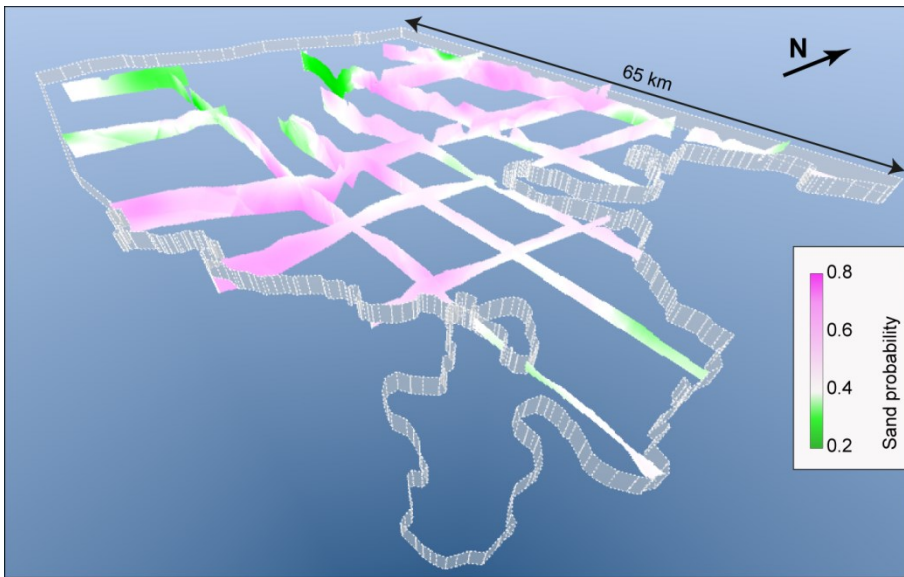


Figure 8: 3D fence view into the sand probability grid, seen from south-east. Vertical exaggeration = 10x.

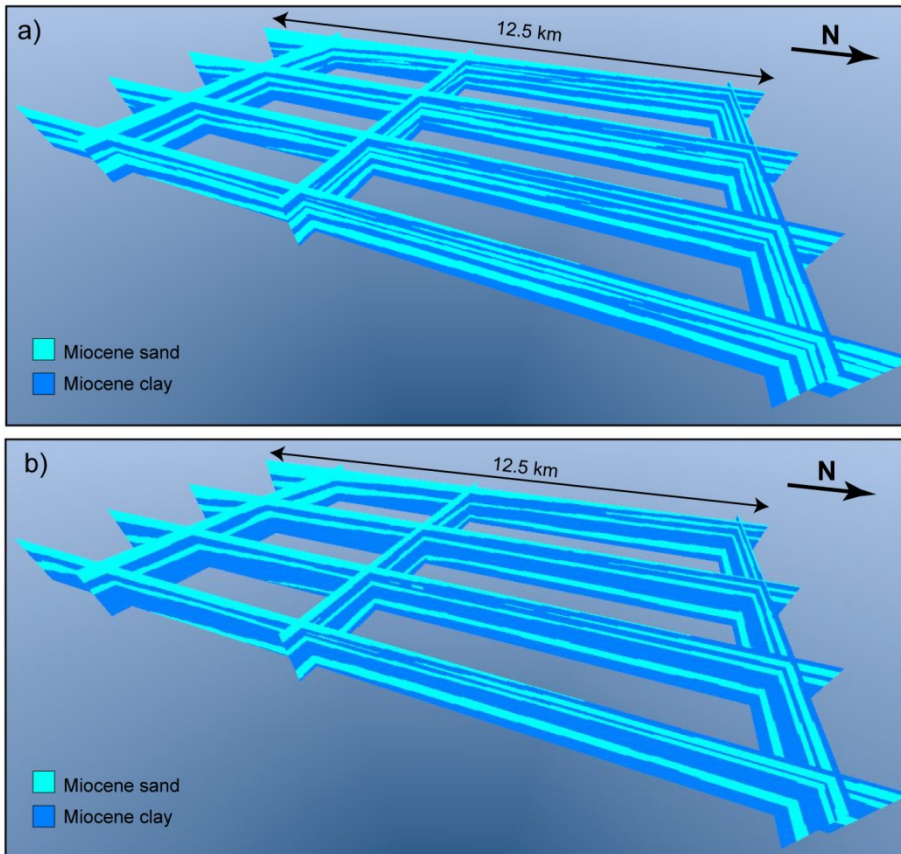


Figure 9: N-S and E-W slices through the two tested 3D training images seen from north-east. a) The first TI (TI1), used to generate the unconditioned realization in Fig. 10a. b) The second TI (TI2), used for the unconditioned realization in Fig. 10b. Vertical exaggeration = 3x.

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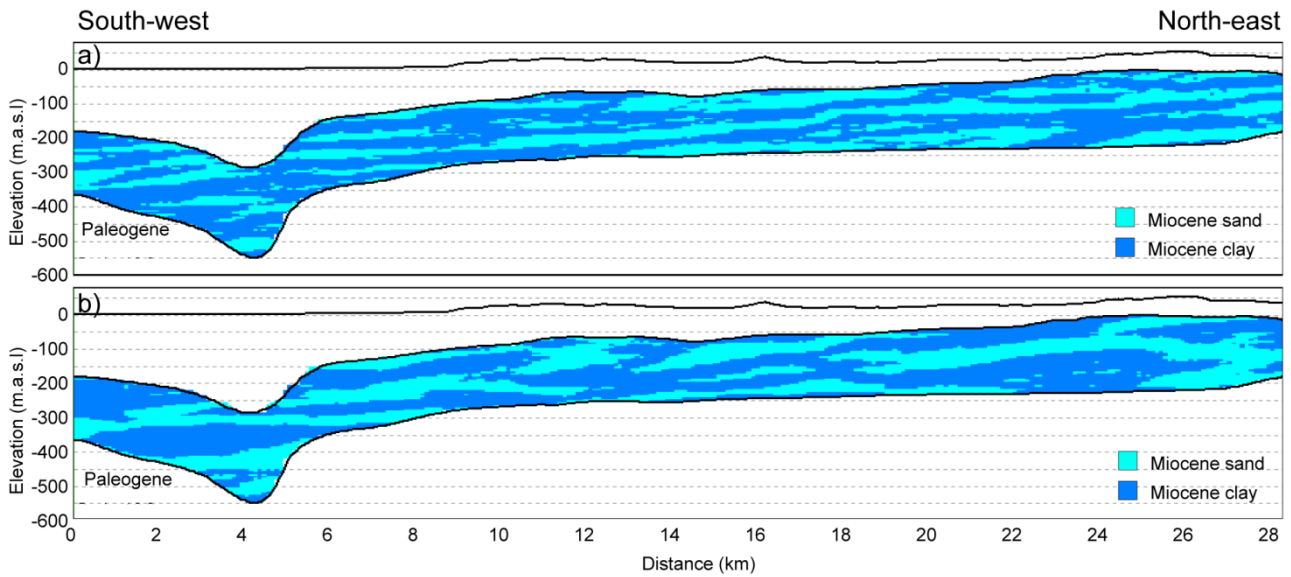


Figure 10: Profile through the unconditioned realizations obtained by using the two different TIs shown in Fig. 4. a) Realization based on **the first-TI1** (Fig. 9a). b) Realization based on **the second-TI2** (Fig. 9b). Vertical exaggeration = 8x. For location of the profile, see **Fig.14Fig. 14**.

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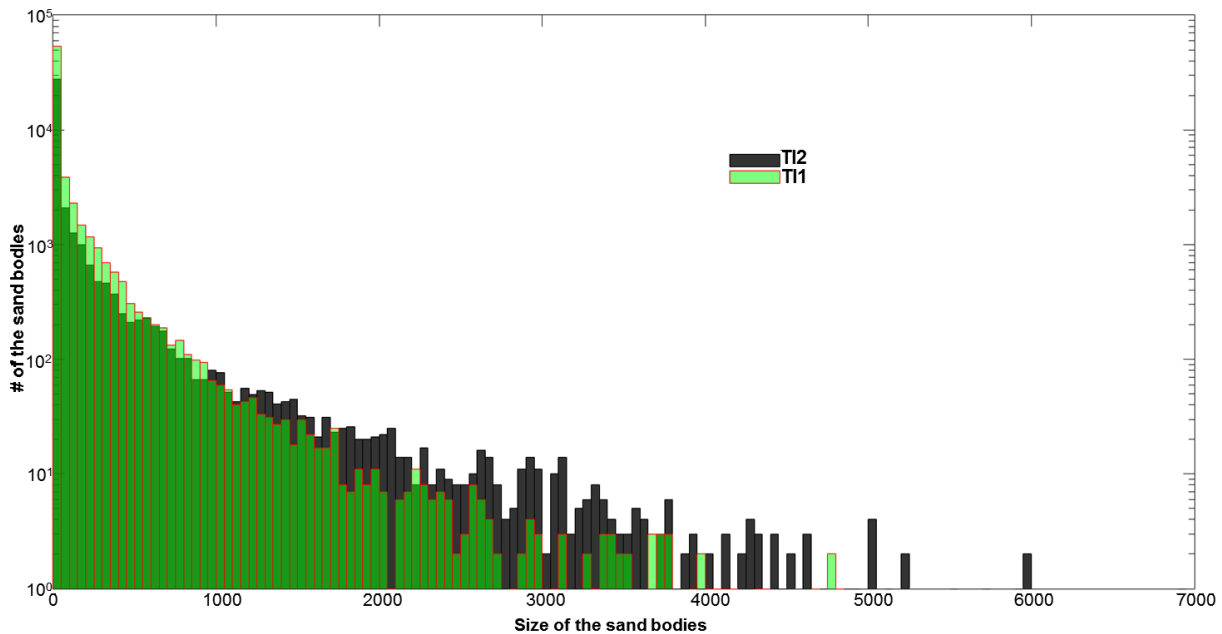


Figure 11: Sizes of the sand bodies of the unconditioned realizations obtained by using the two different TIs shown in Fig. 9.

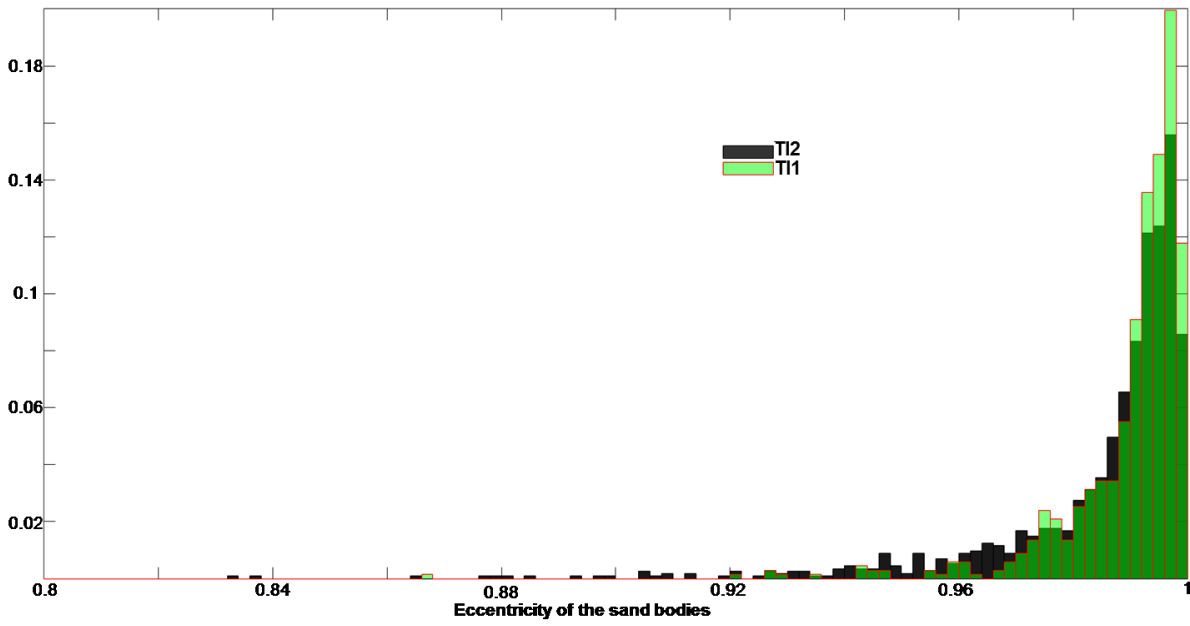


Figure 12: Probability of the eccentricity of the sand bodies (with a size larger than 1000) for the unconditioned realizations obtained by using the two TIs in Fig. 9.

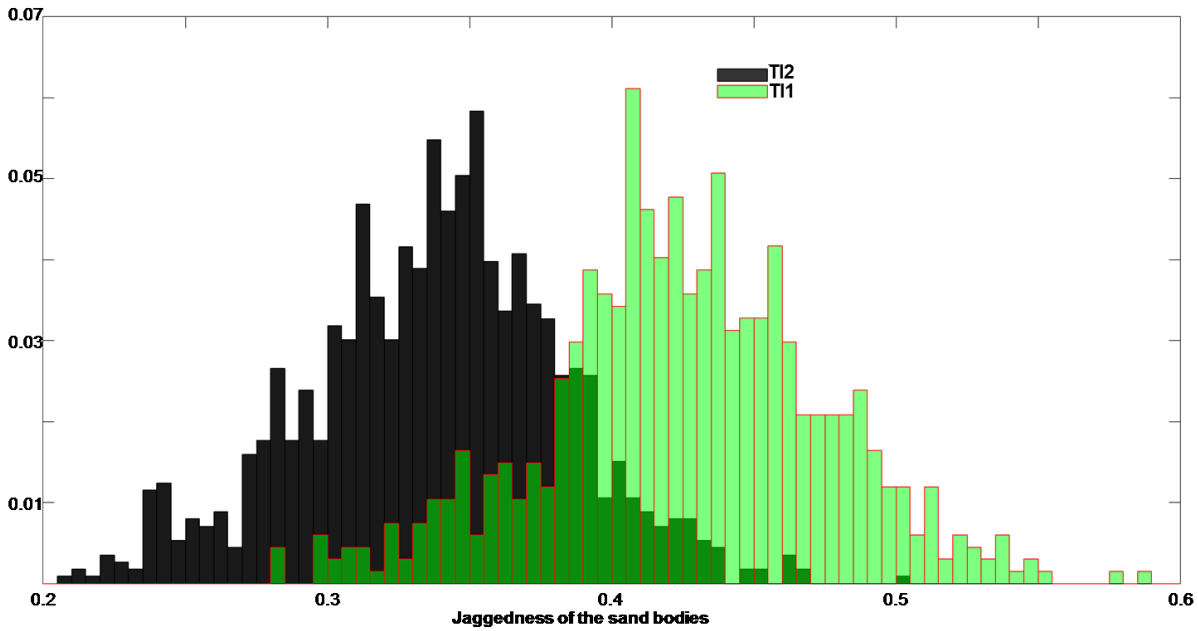


Figure 13: Probability of the jaggedness of the sand bodies (with a size larger than 1000) for the unconditioned realizations obtained by using the T1 and T2 in Fig. 9.

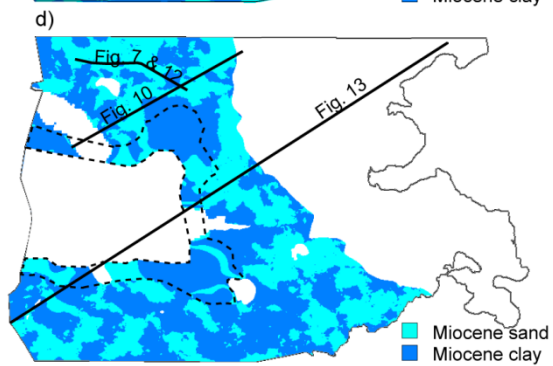
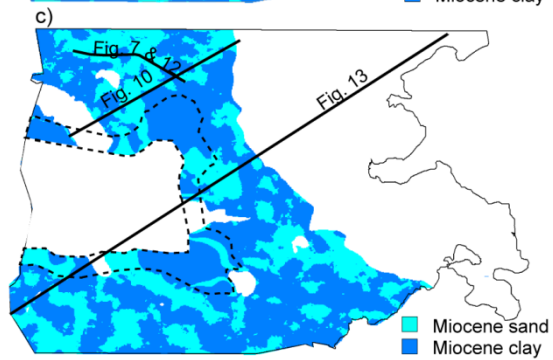
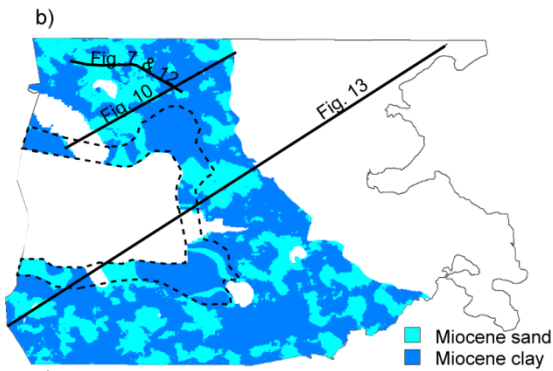
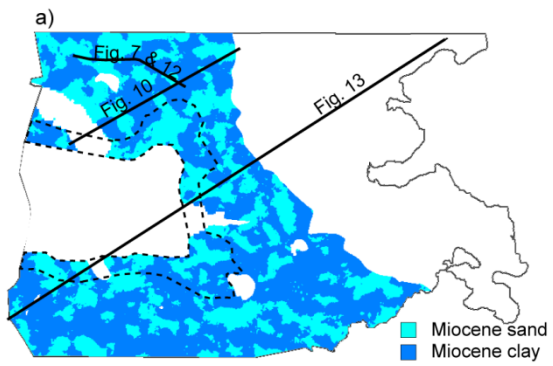
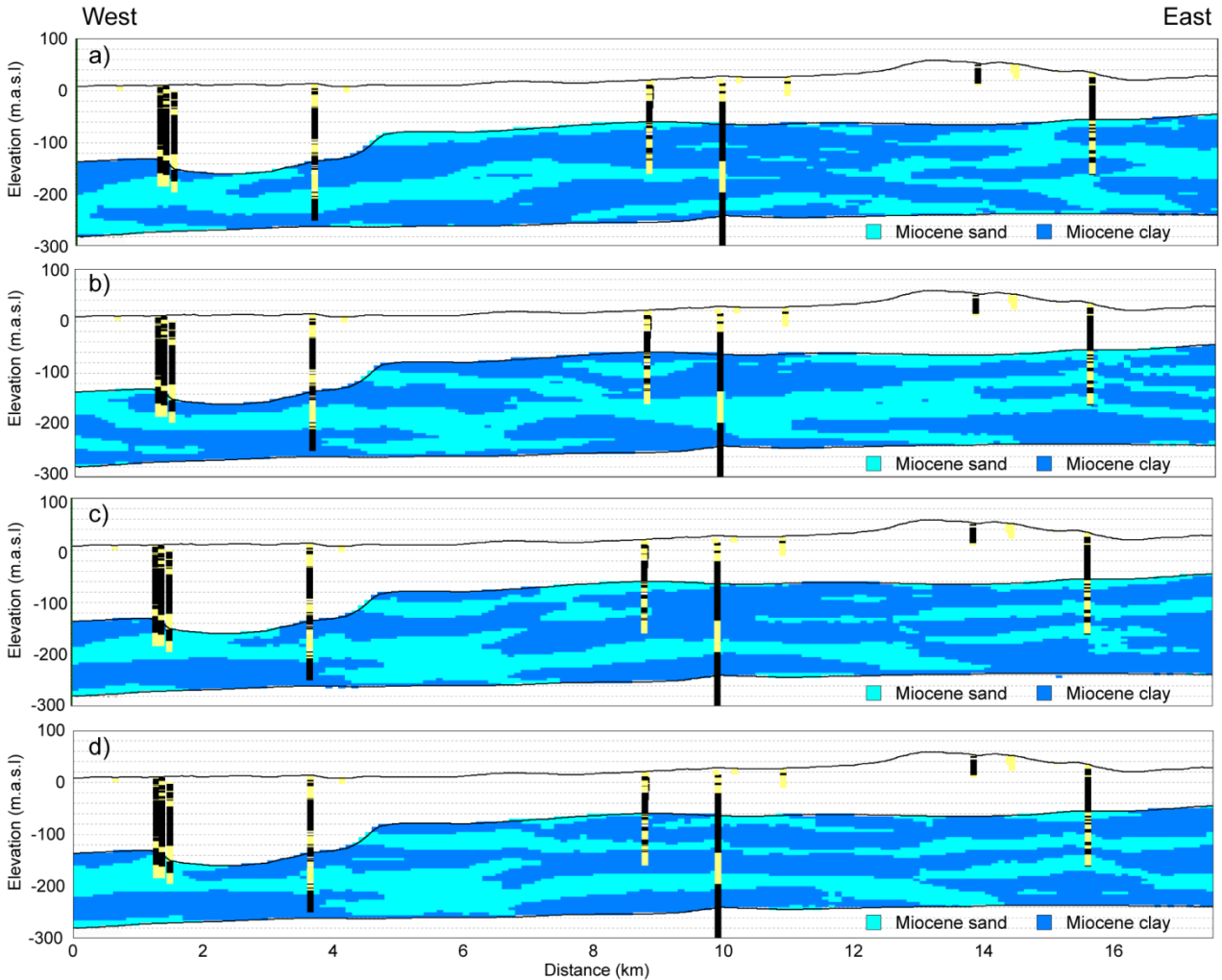


Figure 4.14: Horizontal slice at elevation -188 m through the realizations generated by using different conditional strategies (see Table 1). Position of the profiles in Figs. 7, 10 & 12 and 13 are showed. The dashed region encapsulates the buffer around the Tønder model, which has been used as hard conditioning information in (b), (c) and (d).



5 | Figure 4.15: Profile through the realizations generated by using different conditional strategies (see Table 1). The borehole information used for conditioning is illustrated in Fig. 7: a) unconditioned; b) borehole as hard data (Fig. 7a); c) borehole as soft data (Fig. 7b); d) sand probability grid derived by boreholes as soft data (Fig. 7c). Sand/clay information from the original boreholes are showed within a buffer of 100 m (yellow = sand, black = clay, white = 'other'). For location of the profile, see Fig. 4.14. Vertical exaggeration = 8x.

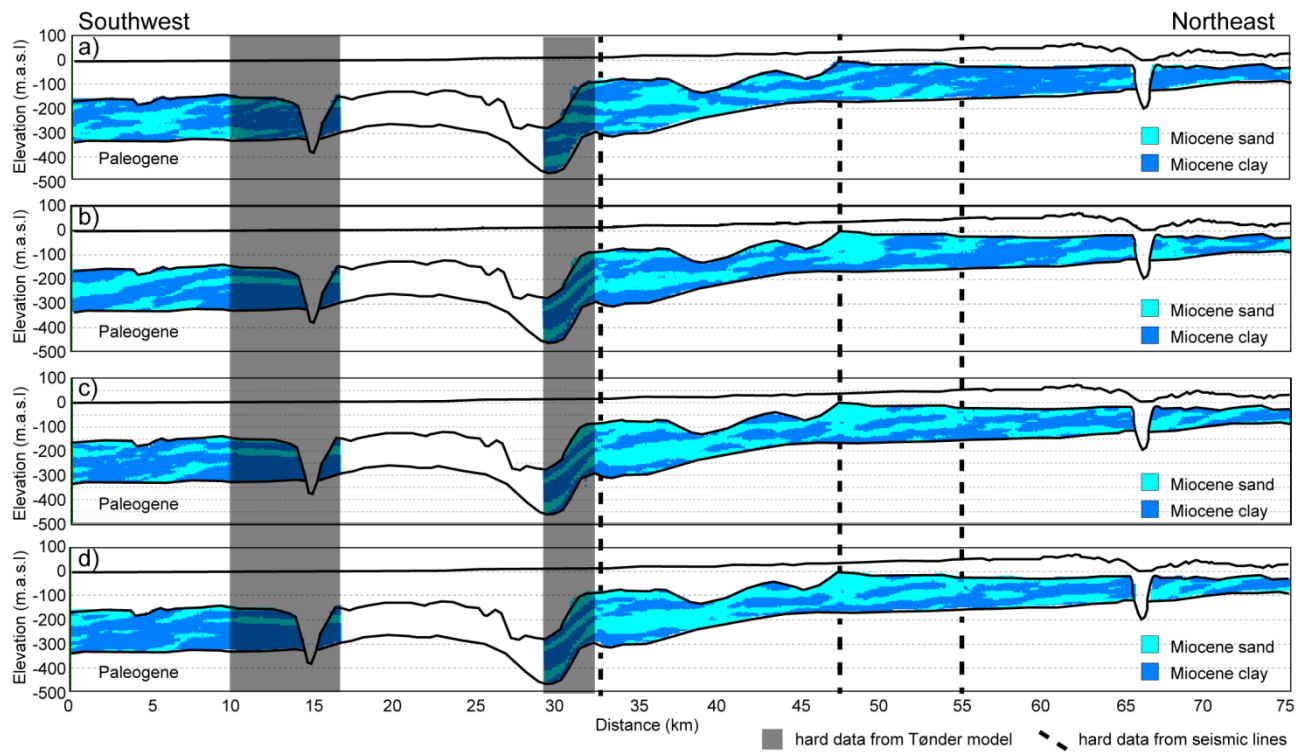


Figure 163: Long SW-NE profile through the realizations generated by using different conditional strategies (see table 1). For location of the profile, see [Fig. 14](#). Vertical exaggeration = 15x.

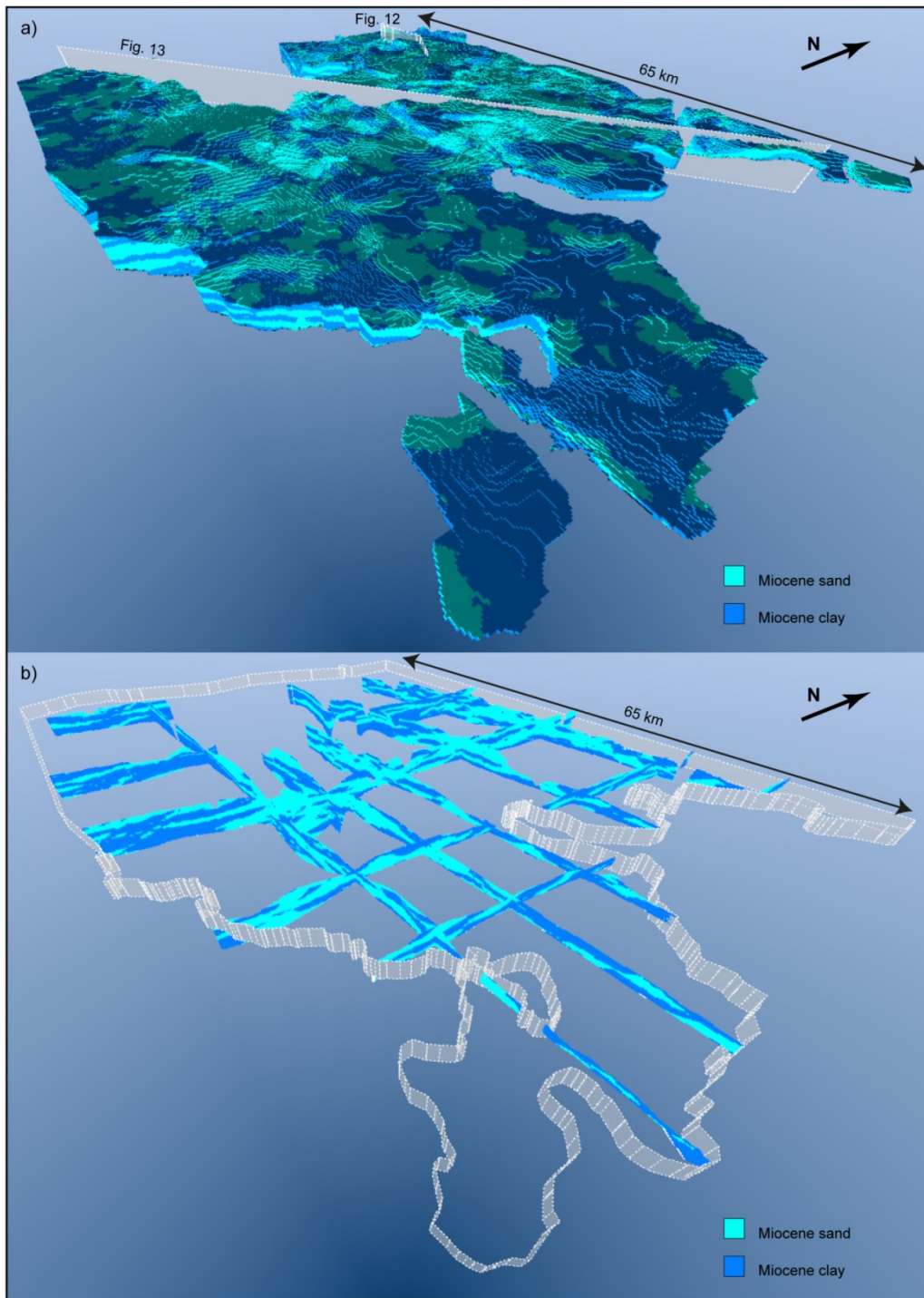


Figure 1417: 3D view of the final realization (test (d), Table 1). The associated 3D probability grid is shown in Fig. 8. a) All voxels are plotted and the location of the profile in Figs. 12 and 13 are shown. b) The associated fence view. Vertical exaggeration = 10x.

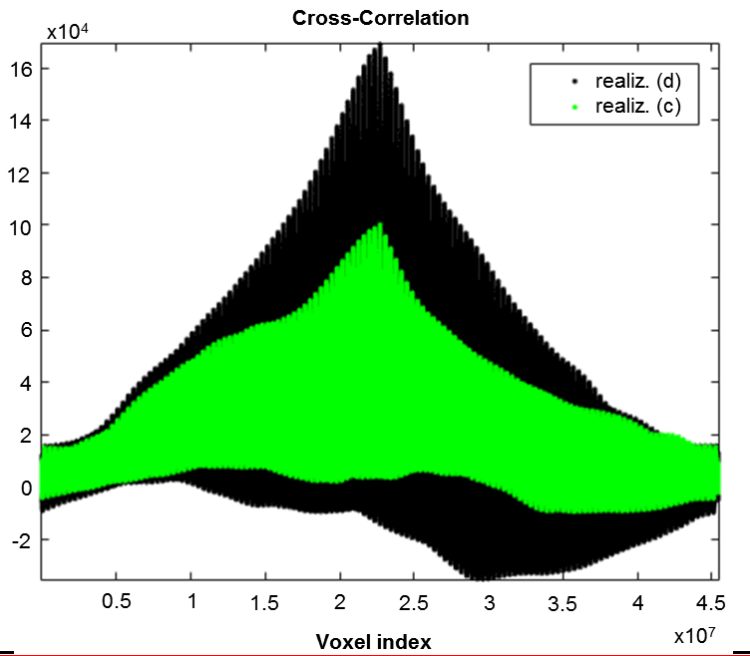


Figure 18: Cross-correlation between the soft probability distribution (Fig. 8) and each of the realizations showed, for example, in Fig. 14c (real. (c)) and Fig. 14d (real. (d)), and described in Table 1 (cases (c) and (d)).

Strategy	Training image	Soft data	Hard data
a	2 nd (Fig. 9b)	÷	÷
b	2 nd (Fig. 9b)	÷	The Tønder model Seismic interpretation Boreholes
c	2 nd (Fig. 9b)	Sand probability directly from boreholes	The Tønder model Seismic interpretation
d	2 nd (Fig. 9b)	3D kriged grid of the sand probability distribution from boreholes	The Tønder model Seismic interpretation

Table 1: The different conditioning strategies tested in this study. The corresponding realizations are presented in the Figs. ~~10~~14-16-12.