



**Challenges in  
conditioning a  
stochastic geological  
model**

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# Challenges in conditioning a stochastic geological model of a heterogeneous glacial aquifer to a comprehensive soft dataset

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## Abstract

In traditional hydrogeological investigations, one geological model is often used based on subjective interpretations and sparse data availability. This deterministic approach usually does not account for any uncertainties. Stochastic simulation methods address this problem and can capture the geological structure uncertainty. In this study the geostatistical software TProGS is utilized to simulate an ensemble of realizations for a binary (sand/clay) hydrofacies model in the Norsminde catchment, Denmark. TProGS can incorporate soft data, which represent the associated level of uncertainty. High density (20 m × 20 m × 2 m) airborne geophysical data (SkyTEM) and categorized borehole data are utilized to define the model of spatial variability and for soft conditioning the TProGS simulations. The category probabilities for the SkyTEM dataset are derived from a histogram probability matching method, where resistivity is paired with the corresponding lithology from the categorized borehole data. A novelty of this study is the incorporation of two distinct datasources into the stochastic modeling process that represents two extremes of the conditioning density spectrum; sparse borehole data and abundant SkyTEM data. The high density of spatially correlated SkyTEM data lead to very deterministic simulation results. This is caused by overconditioning and addressed by a work around utilizing a resampling (thinning) of the dataset. In the case of abundant conditioning data it is shown that TProGS is capable of reproducing non-stationary trends. The stochastic realizations are validated by five performance criteria: (1) sand proportion, (2) mean length, (3) geobody connectivity, (4) facies probability distribution and (5) facies probability – resistivity bias. As conclusion, a stochastically generated set of realizations soft conditioned to 200 m moving sampling of geophysical data performs most satisfying when balancing the five performance criteria and can be used in subsequent hydrogeological flow modeling to address the predictive uncertainty originated from the geological structure uncertainty.

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# 1 Introduction

Constraints in accurate and realistic solute transport modeling hydrogeology are caused by the difficulty of characterizing the geological structure. The subsurface heterogeneity heavily influences the distribution of contaminants in the groundwater system. The available data are often not sufficient to reflect the heterogeneity correctly. As the scale of heterogeneity is often smaller than the data availability (e.g. borehole spacing) a detailed characterization of the heterogeneity can substantially improve the model quality. In traditional hydrogeological studies, one geological model is built based on the best comprehensive knowledge from often sparse borehole data and subjective interpretations. This can lead to alleged correct results, for instance when addressing the water balance on catchment scale, but will often prove to be inadequate for simulations beyond general flows and heads, e.g. contaminant transport modeling. Therefore, it is proposed by numerous studies that the uncertainty on the geological conceptualization is crucial when assessing uncertainties on flow paths (Neuman, 2003; Bredehoeft, 2005; Hojberg and Refsgaard, 2005; Trolborg et al., 2007; Seifert et al., 2008). One of the strategies often recommended for characterizing geological uncertainty and assessing its impact on hydrological predictive uncertainty is the use of multiple geological models (Refsgaard et al., 2012). In this respect geostatistical tools such as TProGS (Carle and Fogg, 1996; Carle et al., 1998) and multipoint statistics (Strebelle, 2002) are powerful tools as they enable the generation of multiple equally probable realizations of geological facies structure. This study targets the realistic description of heterogeneity in a geological model by introducing diverse data into the modeling process with the overall aim to reflect the geological structure uncertainty by generating a set of equally plausible realizations of the subsurface using TProGS.

Geostatistics is able to tackle the above mentioned problem (Refsgaard et al., 2006). Multiple plausible realizations of the geological model are generated, that honor both, the available data and a defined model of spatial variability. Next to TProGS and multi point statistics, sequential Gaussian simulations (Lee et al., 2007) and variogram

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geostatistics (Gringarten and Deutsch, 2001) are widely used to generate subsurface models. TProGS has been successfully applied to simulate highly heterogeneous subsurface systems by constraining the simulation to borehole data (Carle et al., 1998). Weissmann et al. (1999), Weissmann and Fogg (1999) and Ye and Khaleel (2008) use additional spatial information obtained from soil surveys, sequence stratigraphy and soil moisture, respectively for accessing the complex lateral sedimentary variability and thus improving the quality of the model of spatial variability. Recent studies by Lee et al. (2007) and dell’Arciprete et al. (2012) highlight that TProGS is compatible with other geostatistical methods like, multi-point statistics, sequential Gaussian simulations and variogram statistics. The distinct strength of TProGS is the simple and direct incorporation of explicit facies manifestations like mean length, proportion and (asymmetric) juxtapositional tendencies to other facies.

In TProGS field observations can constrain the simulation as soft or hard conditioning. “Hard conditioning” forces the realizations to honor data completely whereas “soft conditioning” honors the data partly in respect to the uncertainty of the observation (Falivene et al., 2007). This feature is essential because it enables the user to associate uncertainties to the conditioning dataset that can be of either subjective or objective nature. The information on geological structures can be greatly improved by applying geophysical methods, such as SkyTEM (Christiansen and Christensen, 2003; Jorgensen et al., 2003b; Sorensen and Auken, 2004; Auken et al., 2009), an airborne transient electromagnetic method. This study utilizes a method that translates SkyTEM observation data into facies probability which enables to associate the geophysical data with softness, according to the level of uncertainty.

Until now there are no published studies on the incorporation of a comprehensive and continuous soft conditioning datasets to a stochastic simulation such as TProGS. Alabert (1987) published an early study on the implications of sparse soft condition data to a stochastic simulation (SIS). The analysis shows that soft conditioning significantly increases the quality of the realizations. The same observation is presented by McKenna and Poeter (1995), where soft condition data, derived from geophysical

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measurements could significantly increase simulation performance. It has not been tested whether stochastic models, especially TProGS, are capable of handling abundant soft conditioning data. Moreover, the risk that a cell-by-cell soft dataset may cause an overconditioning of the simulation has not been fully investigated.

Geophysical datasets are valuable information in many hydrogeological investigations. It can considerably improve the conceptual understanding of a facies or hydraulic conductivity distribution and identify non-stationary trends. Stationarity assumes that the same statistical properties are applicable over the entire domain. Seifert and Jensen (1999) approach the problem of simulating a non-stationary system in TProGS by subdividing the simulation domain into stationary sub-domains with independent models of spatial variability and hard conditioning along the seamlines to ensure good connectivity. We are not aware of stochastic studies focusing on non-stationarity that tests if a comprehensive soft conditioning dataset representing the observable non-stationary trends is capable of reproducing these accordingly.

Most stochastic studies only make relatively simple validations of how well the simulations are able to reproduce known geostatistical properties. Carle (1997) and Carle et al. (1998) investigate the goodness of fit between the simulated and the defined spatial variability. The geobody connectivity is used by dell’Arciprete et al. (2012) to compare results originating from two- and multipoint geostatistics. However no guidance on which performance criteria to use and how to conduct a systematical validation of a stochastic simulation exists. Complex stochastic simulations using comprehensive conditioning datasets pose additional challenges in this respect.

The objectives of this study are: (1) to setup TProGS for a study site based on lithological borehole data and high resolution airborne geophysical data and investigate the effect of the two distinct conditioning datasets to the simulation; (2) to assess the problem of overconditioning in a stochastic simulation; (3) to ensure that non-stationary trends are simulated accordingly by TProGS; and (4) to identify and test a set of performance criteria for stochastic simulations that allow the validation of simulation accuracy against geostatistical properties derived from field data. The results of the present

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study are intended for application in a hydrological modeling context (Refsgaard et al., 2014).

## 2 Study site

Figure 1 shows the 101 km<sup>2</sup> Norsminde catchment, located on the east coast of Jutland south of Aarhus. The topography allows a separation between an elevated western part, with changing terrain and a maximum elevation of 100 m and a flat and low elevated eastern part, where the coastline represents the eastern boundary. Glacial morphologies, namely moraine landscapes are predominant in most of the catchment. Gravel, meltwater-sand and clayey and sandy tills are prevalent in the Norsminde catchment. The stratigraphy consists of an upper layer of glacial sediments, varying in thickness between 10 and 40 m. Lithological borehole descriptions from this layer indicate an alternating facies distribution of sand and clay. The thickness of the sand lenses varies from less than a meter to 20 m. A layer of Miocene sediments lies beneath the glacial sediments and consists of a heterogeneous sand and clay system. Below is a sequence of Paleogene clay, which is characterized by very plastic properties and very low hydraulic conductivity. This study focuses on the stochastic simulation of a delineated glacial structure in the western part of the Norsminde catchment. It provides interesting challenges like distinct heterogeneity and a diverse terrain.

## 3 Data

Two different sources of data, namely lithological borehole data and airborne based geophysical data (SkyTEM) are used, where the former is utilized to describe the vertical sand and clay variability and the latter for assessing the lateral direction.

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### 3.1 Borehole data

The borehole dataset contains 112 borehole logs with varying depths. The descriptions in the borehole reports are converted to a categorical binary (sand/clay) system at 5 cm vertical discretization. Further each borehole's uncertainty is validated (He et al., 2013). The uncertainty assessment allows defining individual trust scores and thus the definition of how much each borehole should constrain the conditional simulation in the form of soft data. Drilling method, age, purpose of drilling, among others are used as variables to ensure a systematic approach to validate the uncertainty of each individual borehole. The boreholes are grouped into four quality groups with 100, 95, 90 and 85 % as trust scores. The classified borehole dataset states an overall sand proportion of 30 %.

### 3.2 Geophysical data

The geophysical dataset comprises resistivity data from SkyTEM helicopter surveys. The SkyTEM method has been extensively used for subsurface mapping in Denmark (Jorgensen et al., 2003a, 2005), where it has proven to be a successful tool for hydro-geological investigations. SkyTEM data have the advantage of a high spatial resolution in the top 20 to 30 m and at large spatial coverage. However, some studies rise concern about the accuracy of interpretations of deep soundings (Andersen et al., 2013). In the Norsminde catchment data were collected at 2000 flight km containing over 100 000 sounding points. The distance between the flight lines is between 50 and 100 m. The dataset is processed with a spatially constrained inversion algorithm (Schamper and Auken, 2012) giving a 3-D distribution of the underground resistivity. The sounding data were interpolated to a 20m × 20m × 2 m grid domain by using 3-D kriging as the interpolation method. The gridded resistivity data can be utilized as a proxy for lithology, as high and low resistivity cells indicate a high probability of sand and clay, respectively. The SkyTEM dataset covers approximately 85 % of the delineated glacial sequence. Figure 2 shows the spatial variation of the median resistivity for a 4- and a 16- subarea

grid. Higher median resistivity values are located in the southern part of the glacial sequence. This indicates a greater sand proportion in the given areas. The conclusion of the spatial pattern in Fig. 2 is that stationarity cannot be attested to the glacial sequence. This will have implications for the stochastic simulation.

The exact sand proportion can be derived by introducing a cut off value that divides the SkyTEM dataset into a sand and a clay fraction. Jorgensen et al. (2003b) estimate resistivity thresholds to differentiate between sediments in buried valleys in Denmark. Accordingly, glacial sand has a resistivity greater than 60  $\Omega\text{m}$  whereas clayey till sediments are placed between 25 and 50  $\Omega\text{m}$  and thus the exact cut off value varies between study sites. He et al. (2013) developed a method to manually calibrate the cut off value by comparing borehole with SkyTEM data at different spatial domains with the aim to reduce the deviation in sand proportion between the two data. It is assumed that the deviation has to be minimized at domains with a high borehole density where the boreholes are assumed to best represent the domain conditions. It is shown that a borehole density of 2 per  $\text{km}^2$  reduces the representative error and that 46  $\Omega\text{m}$  as cut off value reduces the deviation in sand proportion between the two datasets. The calibrated cut off value yields a sand proportion of 23 %.

Further He et al. (2013) developed a histogram probability matching method that enables a direct translation from resistivity into facies probability. Resistivity is paired with the lithological borehole description at the coinciding cell. The data pairs are grouped in 10  $\Omega\text{m}$  bins and for each bin the sand/clay fraction is first calculated and then plotted as a histogram. 3rd order polynomial curve fitting is applied to the histogram and the manually calibrated cut off value is superimposed to the fitted curve (Fig. 3). The shape of the curve reflects the combined uncertainties from both datasets. The flatness of the transition zone, around 50 %, sand probability indicates a high uncertainty for the corresponding resistivity values.

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4 Methods

4.1 TProGS – Transition Probability Geostatistical Software

The geostatistical software TProGS is applied in this study. It is based on the transition probability (TP) approach (Carle and Fogg, 1996; Carle et al., 1998). Continuous Markov Chain models (MCM) are used to represent the model of spatial variability (Krumbein and Dacey, 1969; Carle and Fogg, 1997; Ritzi, 2000). TProGS allows for the simulation of multiple realizations by utilizing a sequential indicator simulation (SIS) (Seifert and Jensen, 1999) and by performing simulated quenching (Deutsch and Cockerham, 1994; Carle, 1997). These two steps are mutual dependent and they make sure that the realizations honor local conditioning data as well as the defined model of spatial variability.

The major advantage of TProGS is that fundamental observable attributes are parameterized in the modelling process: volumetric fractions (proportions), mean lengths (thickness and lateral extent) and (asymmetric) juxtapositional tendencies. These attributes can be assessed by data analysis and geological interpretations and control the shape of the MCM model. The facies proportion is related to the asymptotic limit of the MCM. The mean length is indicated on a plot of auto-transition probabilities as the intersection of the tangent at the origin with the  $x$  axis. Asymmetric juxtapositional tendencies are of interest when simulating a system with at least three categories and can thus be neglected in this study. TProGS computes the realizations of the geology in two uncoupled, but mutually dependent steps. An initial configuration of facies distribution is produced by the SIS algorithm (Deutsch and Journel, 1992). Secondly, the initial configuration is reshuffled by the simulation quenching optimization algorithm (Deutsch and Cockerham, 1994). The TProGS simulation domain of this study is discretized into  $20\text{ m} \times 20\text{ m} \times 2\text{ m}$  cells on a  $450 \times 600 \times 40$  cell grid. The horizontal transition probabilities (TP) are based on SkyTEM data, that is categorized by a cut off value of  $46\text{ }\Omega\text{m}$  and the vertical extent is purely based on borehole data.

## 4.2 Split sample test

The two incorporated conditioning datasets are very distinct and will affect the simulation in opposite ways: sparse borehole data allow large simulation freedom whereas dense SkyTEM data limit the simulation freedom. Naturally they will be combined in order to condition the simulation to the best combined knowledge of the system. However it is of interest to know how each individual conditioning dataset affects the simulation. In this context a split sample test can reveal valuable information: one simulation conditioning to purely borehole data and the other one conditioned to purely SkyTEM data. It will be tested how well the simulations conditioned to borehole data reproduce the high resistivity cells, where a high sand probability is evident and how well the simulations conditioned to SkyTEM data reproduce the locations with borehole information.

## 4.3 Moving sampling

Most studies on stochastic modeling condition the simulation to sparse data. In this study a comprehensive cell-by-cell soft conditioning dataset is applied and it is anticipated that this may result in overconditioning, because the correlation length is much larger than the cell length. Thinning the conditioning dataset out is a very intuitive sampling approach to work around the problem of overconditioning. However, if the resampled conditioning dataset is too sparse, information from the original dataset might not be sufficiently accounted for. Opposed to the static sampling technique a moving sampling method, where different location grids are sampled in a systematic way to build the conditioning datasets, ensure that most possible original information is retained in the resampled soft conditioning dataset. For this study five different soft datasets are extracted, all equipped with the same sampling distance between data. Five realizations are computed for each soft dataset; giving a total of 25 realizations. In addition to the comparison between moving and static sampling, different sample densities will also be tested.

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## 4.4 Sampling scenarios

In total, eight conditioning scenarios are tested in this study. For the split sample test two scenarios are used, namely purely borehole data (“*onlyBH*”) and purely cell-by-cell SkyTEM data (“*onlySky20*”). In the following both datasources are combined to represent the optimal combined knowledge of the system. Further, static and moving sampling are applied: Borehole data and SkyTEM data sampled statically at 20, 100, 200 and 500 m (“*BH-Sky20static*”, “*BH-Sky100static*”, “*BH-Sky200static*” and “*BH-Sky500static*”, respectively). Moving sampling is tested at 100 and 200 m sampling distance (“*BH-Sky100moving*” and “*BH-Sky200moving*”, respectively).

## 4.5 Performance criteria

The simulation domain of TProGS is rectangular and SIS and quenching ensure that the predefined geostatistical properties (mean length and proportion) are accounted for. However, in reality the simulation target is a 3-D body within the rectangular model domain. Thus the geostatistical parameters may deviate between the simulation target and the entire model domain. The glacial structure in the Norsminde catchment represents only approximately 20 % of the entire TProGS simulation domain and deviations in simulated spatial statistics between the entire model domain and the simulation target are expected.

### 4.5.1 Sand proportion

The deviation between the mean simulated sand proportion and the defined sand proportion in the MCM can be calculated for a set of realizations. The focus should be on the target area only, the area that will be extracted from the rectangular model domain for subsequent applications. The analysis of the sand proportion is based on 25 realizations.

### 4.5.2 Mean length

The simulated mean length can be estimated by recalculating the TPs from the TProGS output for the target area only. The simulated TPs for a set of realizations can be averaged (10 realizations in this case) and compared with the measured TPs to estimate the deviation in mean length between the predefined and the mean simulated length.

### 4.5.3 Geobody connectivity

The degree of connectivity of permeable areas in the subsurface has major implications for flowlines and particle ages. Renard and Allard (2013) conducted a methodology study on various static and dynamic connectivity metrics. These metrics can be utilized as a comparison and interpretation indicator for multiple stochastically generated realizations of the geology. The work by dell'Arciprete et al. (2012) shows the successfully implementation of connectivity metrics to compare stochastic realizations computed by two- and multi-point statistics.

For this study two static connectivity metrics,  $\theta$  and  $\Gamma$ , are selected. They refer to the first and second geobody connectivity defined by Hovadik and Larue (2007). A geobody is defined as one connected 3-D cluster of the same facies.

$$\theta = \frac{V_l}{\sum_{i=0}^n V_i} \quad (1)$$

$$\Gamma = \frac{\sum_{i=0}^n (V_i)^2}{(\sum_{i=0}^n V_i)^2} \quad (2)$$

where  $V_i$  is the volume of an individual geobody,  $n$  is the number of unconnected geobodies and  $V_l$  is the volume of the largest occurring geobody.  $\theta$  represents the ratio of the volume of the largest geobody to the total volume. Denoted as  $\Gamma$  is the proportion of

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the pairs of cells that are connected among the entire pairs. The two selected connectivity metrics originate from the percolation theory, which describes the transition from many disconnected clusters to one large coherent cluster. This is mainly depending on the facies proportion. As the proportion gradually increases it reaches a point where

one big cluster appears. The percolation threshold is expected to be approximately 0.59 and 0.31 for a 2-D and 3-D grid, respectively (Hovadik and Larue, 2007). Mean values of  $\theta$  and  $\Gamma$  are computed based on 10 realizations.

#### 4.5.4 Facies probability distribution

The facies probability distribution reflects the inter variability among a set of realizations and can be extracted from a probability map. Each cell in the probability map reflects the simulated category probability within a set of realizations. The comparison between the distribution of the original soft dataset, which constrains the simulation and the simulated facies probability distribution, allows validating the performance of the simulation. Ideally the distribution of the original soft dataset is reproduced by the simulation, which does not allow assumptions concerning the accuracy of the allocation pattern of the simulated facies probability.

#### 4.5.5 Facies probability – resistivity bias

The validation of the facies probability – resistivity bias depicts if the simulated facies probability corresponds to the fitted curve derived from the histogram probability matching method, and thereby test whether the simulated facies probability is according to the resistivity pattern. The simulated facies probability value is paired with the coinciding resistivity value of the gridded SkyTEM dataset. The pairs are grouped in 5  $\Omega\text{m}$  bins and the median values of simulated facies probability can be plotted for each bin. Further the RMSE can be calculated between the simulated facies probability and the fitted curve at each bin in order to quantify the agreement.

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## 5 Results

### 5.1 TProGS setup

The computed transition probabilities (TP) and the fitted Markov Chain model (MCM) for both horizontal and vertical direction are given in Fig. 4. A sand proportion of 23 % and a mean length of a sand lens of 5 and 500 m for vertical and horizontal direction respectively yield MCMs that are in good agreement with the measured TPs. Figure 2 indicates an increasing gradient in sand proportion from north to south. This non-stationary trend is also shown in Fig. 4 where the additional sand-sand transition MCMs are plotted that fit measured TP data from the northern and southern subdomain; defined by 13 %, 2 m, 400 m and 30 %, 5 m and 600 m respectively. 25 realizations are generated based on the MCMs that are specified in Fig. 4.

### 5.2 Split sample test

Two sets of 25 realizations are computed. The entire conditioning dataset is split into two parts, in order to analyze the effect of both extremes of the conditioning spectrum: Abundant data (*onlySky20*) and sparse data (*onlyBH*).

#### 5.2.1 Visual comparison

Figure 5 presents two individual realizations (a) and (b) and the resulting probability maps (c) and (e) from both conditioning datasets at an elevation of 49 m. Examining the individual realizations reveals that the spatial variability is much greater for the *onlyBH* scenario results. This is reasonable, because the amount of constraining data is also much less. This conclusion is supported by the probability maps. The probability map computed from the *onlySky20* conditioning scenario shows only little inter variability among the 25 realizations and resembles almost a deterministic image. The *onlyBH* scenario simulates a probability map that shows high inter variability among the computed realizations, but the high probable sand areas do not coincide with the

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high resistivity areas in the SkyTEM data (d), because many large sand features are not captured by borehole data. On the other hand, some high probable sand features in the *onlyBH* scenario are not represented by the *onlySky20* scenario, because small sand features that are indicated by the borehole data are not detected by the SkyTEM survey.

### 5.2.2 Quantitative comparison

High resistivity areas are defined by a minimum resistivity value of 60  $\Omega\text{m}$  which is equivalent to 70 % probability of sand occurrence based on the fitted histogram curve in Fig. 3. The results of the split sample test are given in Table 1. The *onlyBH* scenario allocates only 20.1 % of the high resistivity cells accordingly. Also, only 74.3 % of the cells, where the lithology in the borehole reports shows sand are simulated correspondingly. Some of the borehole data are treated as soft data, which enables the simulation to overwrite the lithological information, during the SIS and the simulated quenching. This will happen especially when sand lenses are very thin and vertically confined by clay. The *onlySky20* scenario simulates 44 % of those cells accordingly and allocates almost all high resistivity cells as sand. However, almost 60 % of the high resistivity cells are simulated with 100 % sand probability. This is in poor agreement with field data, because the fitted histogram curve does not exceed sand probability values higher than 85 % (Fig. 3). The SkyTEM dataset indicates a large high resistivity cluster in the south-west at an elevation of 49 m (Fig. 5), which is not detected at all by the borehole dataset, because there is only one borehole penetrating this area.

### 5.2.3 Local comparison

Figure 6 shows the vertical profile of one borehole (99.918) that penetrates the sand cluster and compares the simulation results from the *onlyBH* and *onlySky20* scenarios. The borehole has a trust score of 95 %. While both datasets agree on the top layer being sandy and the occurrence of a thick clay layer below 75 m followed by a sand layer,

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they disagree on the location of the deeper sand layer. In the borehole data this sand deeper sand layer is detected at an elevation of 45 m and below, whereas the SkyTEM dataset indicates sand occurrence approximately 8 m higher; 53 m and below. This discrepancy between 45 and 53 m has considerable implications for the simulation results at 49 m shown in Fig. 5. However, one borehole alone will not be sufficient to substantially influence the simulation over large areas. Marginal amplification of the *onlyBH* scenario is noticeable at borehole 99.918. On the other hand, sand probabilities are clearly amplified in the *onlySky20* scenario; everything above 0.5 is amplified close to 1.0 and everything below 0.5 close to 0. The results from Table 1 and Figs. 5 and 6 support the assumption of overconditioning caused by the comprehensive cell by cell soft conditioning.

### 5.3 Overconditioning

The observed problem of overconditioning is caused by spatially correlated data which are incorporated into the modeling process. A very intuitive approach to work around the problem of overconditioning is thinning of the SkyTEM dataset by only sampling part of it. This will only be necessary in horizontal direction because the correlation length of the data is much less in the vertical direction. There is a tradeoff between the correctly simulated facies probability and the accuracy of the spatial allocation pattern. To illustrate this tradeoff three resampled conditioning scenarios are compiled: 100, 200 and 500 m sampling distance in *X* and *Y* direction and at the same time also including the boreholes for conditioning. For each of the three conditioning scenarios (*BH-Sky100static*, *BH-Sky200static* and *BH-Sky500static*, respectively) 25 realizations are computed and the probability maps for sand are presented in Fig. 7. The simulated probability maps of the *BH-Sky100static* and *BH-Sky200static* conditioning scenarios are visually almost identical. Therefore only the latter is shown (d) and the image is already less deterministic than the results by the *BH-Sky20static* scenario (c). Reducing the conditioning data density increases the uncertainty of sand or clay. But at the same time the accuracy of correctly locating sand or clay units decreases, because the

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*BH-Sky500static* scenario (e) shows high probable sand areas which are not indicated by the original dataset (b). If for instance a high resistivity cell embedded in low resistivity cells is sampled for the conditioning, this cell may generate a sand lens in the out thinned conditioning scenario but would be limited by the neighboring cells in the *BH-Sky20static* scenario. The moving sampling method can improve the spatial coverage of the conditioning datasets and thus improve the quality of a set of realizations.

Again, the high resistivity cells are investigated to analyze if the bigger sand lenses are simulated correctly by the different conditioning datasets (Table 2). It is evident that the percentage of deterministically simulated cells falls drastically after thinning the soft data out. The 100 m distance scenarios still allocates more than 80 % of the high resistivity correctly. On the other hand, the *BH-Sky500static* performs poorly, by only simulating 32.7 % of the high resistivity cells correctly. It is also evident that the differences between static and moving sampling are small with regard to the correct allocation of the higher resistivity cells.

## 5.4 Performance criteria

For further validation of the different sampling distances (20, 100, 200 and 500 m) and sampling schemes (static and moving) the five identified performance criteria will be applied to quantify the quality of the simulations.

### 5.4.1 Sand proportion

Table 3 shows the defined sand proportions of the delineated glacial structure. In order to investigate non-stationarities the model domain is additionally subdivided into north and south. The SkyTEM dataset indicates a higher sand fraction in the southern part compared to the north, 30 and 13 % respectively. The simulated sand proportions for the *BH-Sky20static* scenario show a good agreement with the defined values. Larger deviations are evident for the *BH-Sky200moving* scenario. Both conditioning scenarios are capable of reproducing the non-stationarity of the system, in regard to the sand

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proportion. The sand proportions are somewhat overestimated for *BH-Sky200moving* scenario, and much less for the *BH-Sky20static* scenario. Also the overestimation of simulated sand proportion in the northern subarea is larger than in the southern sub-area.

5.4.2 Mean length

The comparison of the early (first lag = 100 m) measured and simulated TPs for the sand-sand transitions in *X* and *Y* direction allows to validate how well the lateral mean length is simulated by TProGS. Figure 8 comprises the measured TPs in horizontal direction, the fitted MCM and the computed mean TPs for the *BH-Sky20static* scenario and *BH-Sky200moving* scenario, based on 10 realizations, for the total and the sub-domains. The effect of overconditioning is very evident, as the computed mean TPs based on 20 m sampling conditioning data purely represent the original measured TP values. Since no simulation freedom is present, the MCM cannot control the output. On the contrary, the *BH-Sky200moving* scenario computes mean TPs that are more independent from the original data and rather follow the defined MCM. The mean length of a sand lens can be derived by the steepness of the tangent where the lag approaches zero. In general, the TP at lag 0 and 100 m are simulated too low; indicating that the simulated mean size of a sand lens is too small. This is more prominent in results by the *BH-Sky200moving* scenario. It is evident that the non-stationarity of the mean length of a sand lens is represented accordingly, although it is undersimulated at all domains.

5.4.3 Geobody connectivity

For the categorized SkyTEM data  $\theta$  and  $\Gamma$  are computed as 98.7 and 99.3 %, respectively. This shows values close to unity and should not be seen as a real reference, rather as a benchmark, because the deterministic picture does not account for any uncertainties. The TProGS simulations based on the two conditioning scenarios both undersimulate the connectivity metrics. The *BH-Sky20static* scenario yields negative

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deviations of 2.1 and 1.1 %, respectively and the *BH-Sky200moving* scenario 2.8 and 1.4 %, respectively. The results indicate that  $\theta$  and  $\Gamma$  show a similar behavior, where  $\Gamma$  appears to be decreasingly greater as the proportion increases. Values close to unity and the very small deviations are in good agreement with the general percolation theory, which sets the percolation threshold to approximately 30 % for 3-D grids (Hovadik and Larue, 2007).

#### 5.4.4 Facies probability distribution

Figure 9 shows the probability distribution for all discussed conditioning scenarios, with static (a) and moving (b) sampling, with 25 realizations in each set. The original soft data distribution has its maximum at approximately 20 % and less than 5 % are deterministic; 0 or 100 % sand probability. The *BH-Sky20static* scenario simulates approximately 70 % of the cells with zero change and thus has an extremely poor fit with the soft dataset and the overconditioning is very prominent. It appears that overconditioning amplifies the conditioning values to the extremes (e.g. 0.6 is simulated as 1.0 and 0.4 as 0.0, Fig. 6). The *BH-Sky500static* scenario reproduces the probabilities from the original soft dataset well, with only approximately 10 % zero change cells. However, the allocation pattern shows small resemblance with the original dataset (Fig. 7b). *BH-Sky100static* scenario gives an intermediate solution, as the probability is better reproduced than with the *BH-Sky20static* scenario, but still, more than 20 % of the cells are simulated purely deterministic. Nevertheless, the *BH-Sky100static* scenario is dense enough to capture the full variability of the system, as indicated by the original SkyTEM dataset. Additionally the results of the *BH-Sky200static* scenario are plotted in (a). The number of purely deterministic simulated cells is decreased to approximately 20 % and the maximum at 20 % sand probability is close to the original soft dataset. Figure 9b compares the static with the moving sampling approach for the 100 and 200 m distance scenarios. The simulated facies probability distribution shows no differences for the static and moving 100 m distance scenarios. However, at 200 m sampling distance,

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the two sampling techniques are distinguishable, as the moving sampling yields fewer deterministically simulated cells than the static sampling.

### 5.4.5 Facies probability – resistivity bias

The results are given in Fig. 10 for the static sampling (a) and the moving sampling approach (b). The strong amplification of the resulting probabilities originating from the *BH-Sky20static* scenario is obvious in (a). The *BH-Sky500static* scenario performs poorly, especially in high resistivity areas, because those areas are not sufficiently covered by the 500m sampling distance. A better fit is represented by the *BH-Sky100static* scenario, because the amplification is much lower than for the *BH-Sky20static* scenario, especially for high resistivity areas. On the other hand, low resistivity areas are more amplified than high resistivity areas. The *BH-Sky200static* scenario gives a satisfying fit with the original fitted curve, especially in high resistivity areas, which indicates that the high probable sand cells are mostly allocated correctly by the model. The simulated facies uncertainty for the low resistivity cells is rather amplified by the *BH-Sky200static* scenario. Figure 10b investigates the simulation differences caused by the static and moving sampling approach. The behaviour is similar to Fig. 9b, because the differences for the 100 m distance scenarios are marginal, while the *BH-Sky200moving* scenario generates a slightly lower facies probability – resistivity bias than the *BH-Sky200static* scenario. The RMSEs between the fitted curve (Fig. 3) and the simulations show that the *BH-Sky200moving* and *BH-Sky200static* sampling conditioning scenarios perform best, both with a RMSE of 0.06. Comparable are the *BH-Sky100moving* and *BH-Sky100static* sampling conditioning scenarios with a RMSE of 0.09 and 0.08, respectively. The *BH-Sky20static* scenario performs poorest with a RMSE of 0.2.

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## 6 Discussion

### 6.1 TProGS setup

Direct transformation of geophysical data, such as SkyTEM, into a deterministic sub-surface model is risky, because too much reliance on geophysical mapping can lead to seriously wrong hydrogeological models (Andersen et al., 2013). The present study incorporates data from both, high resolution geophysical mapping (SkyTEM) and boreholes. Uncertainties are expected in both datasources and the shape of the fitted histogram curve reflects those. High uncertainty is associated with the transition zone; around 50 % sand probability. Although the cut off value that divides the SkyTEM dataset into sand and clay is calibrated, there is a large quantity of high uncertain cells included which make the measured TPs directly dependent on the cut off value. Therefore the facies proportion and mean length are very sensitive to the selection of the cut-off value. As a result, the MCM in the lateral direction, as part of the TProGS setup, is highly dependent on the way the SkyTEM data is treated.

The SkyTEM dataset used in the present study is a 3-D grid of  $20\text{ m} \times 20\text{ m} \times 2\text{ m}$  which was spatially interpolated from soundings with distances of about 17 m and 50–100 m along and between the flight lines, respectively. To reduce the overconditioning problem it might have been preferable to use the direct sounding data instead of the interpolated dataset. A similar effect is achieved by resampling, but here interpolated data with a higher uncertainty than the direct soundings are used. The amount of SkyTEM data strongly exceeds the borehole data; thus if one sand observation in a borehole description is surrounded by mostly low resistivity cells in the SkyTEM data, it can be expected that the sand observation from the borehole will have little or no influence on the simulation.

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## 6.2 Split sample test

The split sample test analyzes the effects of two conditioning scenarios that lie on both extreme ends of the data density spectrum. The integration of high resolution geophysical data covering the entire model domain and borehole data into one model is as such a novelty. Both datasources have advantages and disadvantages: borehole data have a higher data certainty and a finer spatial resolution in the vertical extent to better represent smaller sand features, but are essentially undersampled in the lateral extend. On the other hand, SkyTEM data have a good spatial coverage and therefore the bigger sand features are well represented, but at the same time the data are associated with a higher data uncertainty. At this point, four major sources of uncertainty can be defined: (1) the inversion that transforms the SkyTEM measurement into resistivity, (2) the borehole data, (3) the relationship between lithology and resistivity and (4) the footprint mismatch between small scale borehole data and large scale SkyTEM data. So it is precarious to assume the SkyTEM data as true geology, but it can serve as a reference/benchmark when validating the simulation results. The *onlyBH* scenario does not capture all of the main sand features, which are revealed by the SkyTEM survey: only 20 % of the high resistivity cells, where the resistivity is greater than 70Ωm are simulated correctly. For the *onlySky20* scenario only 44 % of the sand descriptions in the boreholes are simulated correctly, which underlines that the SkyTEM data does not measure the finer sand features correctly. The conducted split sample test does not allow to draw firm conclusions on simulation performance, it rather analyses the agreement between the two dataset propagated through the model.

## 6.3 Overconditioning

The possibility to assign an uncertainty value to an observation data is an essential feature in TProGS. It allows translating uncertainty evaluations into the modeling process. Problems that are associated with spatially correlated data are identified in this study. Correlated data are a common problem in hydrogeological investigations, e.g.

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the incorporation of temporally correlated discharge data or spatially correlated data originating from remote sensing (surface temperature or soil moisture) into the modeling process. We are not aware of previously reported studies where stochastically generated realizations of subsurface systems have been constrained by cell by cell soft conditioning data. Especially, it has not previously been reported how TProGS is able to handle such a conditioning dataset. TProGS stochastically simulates the subsurface facies system by utilizing the two mutually dependent steps SIS and simulated quenching in the *tsim* module. The SIS simulates cells along a random path. At each cell a local probability estimate is computed by cokriging the  $n$  nearest data or already simulated cells. The simulated quenching step incorporates the initial configuration from the SIS. Cells, that are not associated with hard data, are perturbed along a random path and the change in category is accepted if an objective function is reduced. It is not assured if the soft information is considered accordingly for the cokriging of the local probability estimate in the SIS step nor if it is accounted for in the objective function used for the simulated quenching. Work around methods have to be developed to overcome the problems associated with overconditioning. The most intuitive approach is to thin the original soft dataset by resampling only some of the data and to include a moving sampling strategy to account for the spatial variation in the original dataset. Thinning the SkyTEM dataset out and only considering data on a 200 m spaced moving sampling grid gives the most satisfying results.

## 6.4 Non-stationarity

Non-stationarity can be identified by subdividing the SkyTEM dataset (Figs. 2 and 4). It is successfully tested if abundant conditioning data alone is capable of reproducing the observed non-stationary patterns. The simulation domain is divided into north and south and the mean simulated sand proportion and mean length of a sand lens are computed for the sub-domains. The trends are simulated correctly, but the thinner the conditioning data are resampled the closer the alignment between the two sub-domains is. In a situation of sparse data, e.g. only borehole data for conditioning,

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these non-stationary trends cannot be reproduced correctly. Seifert and Jensen (1999) present an approach to model non-stationarity, which might be more suitable for sparse conditioning data. They suggested dividing the model domain into several stationary sub-domains, and each subdomain is then characterized using independent MCMs.

When subdividing the model domain, care must be taken, that no major features are cut, because it is then difficult to model them correctly. This approach was tested in the present study, but results revealed that this method is not easily applicable in situations of abundant conditioning data, because large coherent sand features are cut by the sub-division and could not be simulated adequately.

### 6.5 Performance criteria

Most studies that focus on the stochastic generation of subsurface models do not validate the performance of the simulation results. We identified and tested five performance criteria for validating the model performance.

1. *Sand proportion*: the simulated sand proportions tend to be overestimated by all simulations (Table 3), with a higher overestimation for the sparse conditioning dataset. Artificial conditioning data outside the target area honoring the defined proportion and MCM may help to make the simulation more homogeneous. In that context, continuous hard conditioning outside the simulation target can be tested.
2. *Mean length*: the simulated and measured TPs are compared by Carle (1997) and Carle et al. (1998). Carle et al. (1998) simulate a four category system and the simulated quenching yields a perfect match between the modeled TPs and the defined MCM. On the other hand, Carle (1997) underlines that small deviations are to be expected and shows this by various examples where different SIS and simulated quenching parameters are tested.
3. *Geobody connectivity*: in general the connectivity is partly dependent on the proportion. The sand connectivity for the simulation based on the *BH-Sky200moving*

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scenario is simulated lower and the sand proportion higher in comparison to the results from the *BH-Sky20static* scenario. This means that the geobody connectivity is not fully depending on the proportion in this study. However it is a more feasible performance criterion for proportions far below the percolation threshold, because proportions close to the percolation threshold will automatically be very close to unity.

We used 25, 10 and 10 realizations to compute the first three performance criteria. Computing a moving average shows that the mean converges to  $\pm 2\%$  deviation to the final mean after ca. 15 realizations for the first criterion and after ca. 5 realizations for the second and third criteria, which justifies the selected number of realizations. The two latter criteria incorporate the computed probability map based on 25 realizations. Probability maps proved to be a useful tool to investigate the inter variability among realizations (Alabert, 1987). The results of the *onlyBH* scenario show the highest inter variability and a moving average tested at 10 random locations in the grid shows that after 20 realizations the mean converges to less than  $\pm 20\%$  from the final mean and to less than  $\pm 10\%$  after 23 realizations. These numbers are supposed to decrease as the conditioning data increase and therefore are 25 realizations in the analysis of the two latter criteria justifiable. The availability of a comprehensive soft dataset allows to set a benchmark for the two later criteria.

1. *Facies probability distribution*: this distribution clearly quantifies the problem of overconditioning, because deterministically simulated cells are easily identified. However a good agreement between the simulated facies probability distribution and the original soft dataset does not ensure that the allocation pattern of the simulated probability is correct. This becomes evident when validating the results of the *BH-Sky500static* scenario.
2. *Facies probability – resistivity bias*: this validates if the fitted histogram in the histogram probability matching method is reproduced by the simulation. The simulated facies probability should be in agreement with a corresponding resistivity

observation to ensure that the spatial allocation pattern is simulated correctly. All bins are weighted the same, neglecting the inequality of data in each bin.

Table 4 compiles the five performance criteria for two different TProGS simulations: the *BH-Sky20static*- and the *BH-Sky200moving* scenario. The advantage of using multiple performance criteria is that concentrating on a single criterion may reveal an alleged good result, while another criterion attests a poor performance to the same simulation. Therefore a weighted and balanced analysis of the performance criteria helps to identify the best result. In this study, where abundant data are available, a good performance of the two latter criteria is as important as simulating accurate mean length/proportion. For example, if only considering sand proportion and mean length, it can be argued that the validation favors the *BH-Sky20static* scenario. However both, the facies probability distribution as well as the facies probability – resistivity bias attest poor performance. On the other hand, if interpreting the probability distribution only, it seems that the validation favors the *BH-Sky500static* scenario. Collectively, the conclusion is that the *BH-Sky200moving* scenario generates the overall most balanced results. The stated performance criteria could further be used in a calibration process to identify a resampled conditioning dataset that generates an even more satisfying set of realizations.

## 7 Conclusions

The novelty of this study is the incorporation of a vast conditioning dataset in the stochastic modeling process and the definition and testing of a set of performance criteria to a TProGS simulation. The categorized SkyTEM dataset is used to define the lateral model of spatial variability, whereas borehole data are used for the vertical direction. Care must be taken when integrating two individual datasets into one conditioning dataset, because a good agreement cannot always be granted. Non-stationary geostatistical properties like facies proportions and mean lengths can be identified. It is

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shown that in the case of abundant conditioning data TProGS is capable of reproducing the non-stationary trends. Spatially correlated data causes the problem of overconditioning, where TProGS simulates a rather deterministic picture of the facies distribution and measured facies uncertainties are not reproduced. Resampling the soft dataset and including moving sampling is an intuitive approach to work around the problem of overconditioning. The *BH-Sky200moving* scenario gives the best tradeoff between the simulated facies distribution and the simulated probability – resistivity bias and is also capable of accounting for the non-stationary trends during the simulation. Five performance criteria are identified in this study: (1) sand proportion, (2) mean length, (3) geobody connectivity, (4) facies probability distribution and (5) facies probability – resistivity bias. The strength of these criteria lies in the integration of all individual criteria to find the most balanced results. These performance criteria help to describe and quantify the accuracy of a set of realizations and could be applied in future geostatistical studies to assess the performance of the stochastic simulation.

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**Table 1.** Split sample test showing how many of the high probable sand cells (resistivity  $> 60 \Omega\text{m}$ ) are simulated with corresponding sand probabilities ( $> 70\%$ ) or fully deterministic (probability = 1.0) among 25 realizations. Conditioned to onlyBH and onlySky20. The last column shows how many of the areas that are shown as sand in the boreholes are simulated with sand probabilities  $> 85\%$ .

Conditioning Scenario	Prob. of sand $> 0.7$ AND resistivity $> 60 \Omega\text{m}$	Prob. of sand = 1.0 AND resistivity $> 60 \Omega\text{m}$	Prob. of sand $> 0.85$ AND borehole = sand
onlyBH	20.1 %	1.34 %	74.3 %
onlySky20	99.0 %	59.1 %	44.0 %

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**Table 2.** Proportion of high probable sand cells (resistivity  $> 60 \Omega\text{m}$ ) that are simulated with corresponding sand probabilities ( $> 70\%$ ) or fully deterministic (probability = 1.0) for six conditioning datasets based on 25 realizations.

Conditioning Dataset	Prob. of sand $> 0.7$ AND resistivity $> 60 \Omega\text{m}$	Prob. of sand = 1.0 AND resistivity $> 60 \Omega\text{m}$
BH-Sky20static	97.9 %	63.8 %
BH-Sky100static/ BH-Sky100moving	84.1 %/87,3	10.4 %/10.1 %
BH-Sky200static/ BH-Sky200moving	75.8 %/71.0 %	5.4 %/3.6 %
BH-Sky500static	32.7 %	1.5 %

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**Table 3.** Simulated and defined sand proportions for the total domain and two sub-domains based on two simulations with different soft conditioning datasets (BH-Sky20static and BH-Sky200moving), based on 25 realizations.

Mean sand proportion (%) based on 25 realizations	BH-Sky20static		
	Total	South	North
Defined	23	30	13
Simulated	25.0	30.7	13.8
Deviation	+2.0	+0.7	+1.8
	BH-Sky200moving		
Defined	23	30	13
Simulated	29.3	33.7	21.5
Deviation	+6.3	+3.7	+8.5

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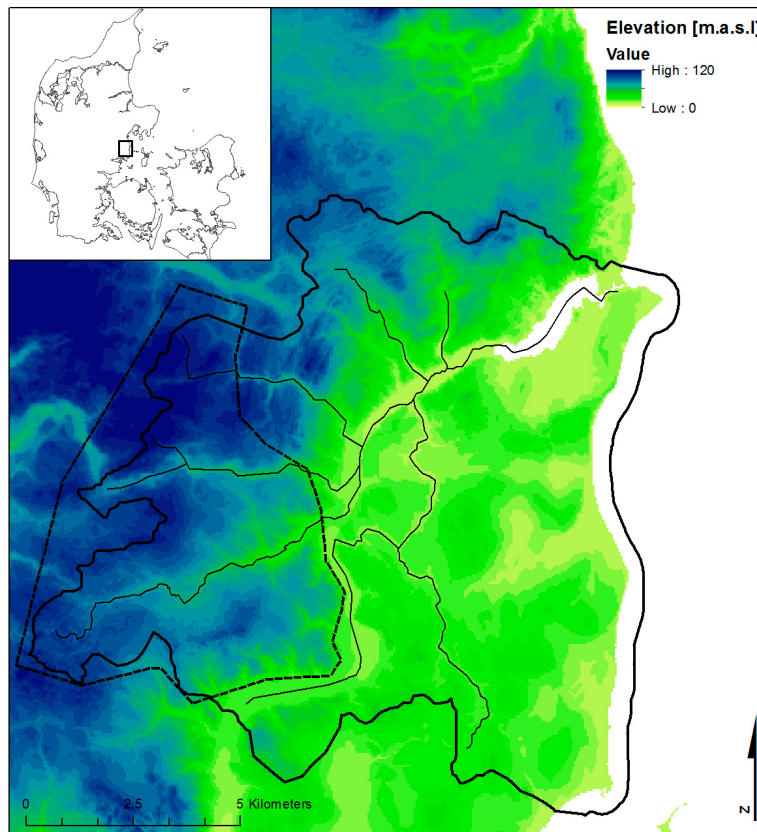
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**Table 4.** The five performance criteria and categorized SkyTEM data as benchmark that are applied to the two simulations with different soft conditioning datasets: cell by cell soft conditioning and 200 m moving sampling soft conditioning; both including borehole data. The first three criteria are expressed as deviation to the benchmark.

Performance Criteria	Categorized SkyTEM	BH-Sky20static	BH-Sky200moving
1. Sand proportion	23 %	+2 %	+6.3 %
2. Mean length (X/Y)	500 m	−21 %/−20 %	−37 %/−37 %
3. Geobody Connectivity ( $\theta/\Gamma$ )	98.7 %/99.3 %	−2.1 %/ − 1.1 %	−2.8 %/ − 1.4 %
4. Facies probability distribution	n.a.	Poor (approx. 70 % cells with zero change)	Satisfying (approx. 15 % cells with zero change)
5. Facies probability-resistivity bias	n.a.	0.20	0.06



**Fig. 1.** The study site in eastern Jutland, Dk. The Norsminde catchment with the delineated glacial structure in the western part of the catchment. Additionally the river network and the topography.

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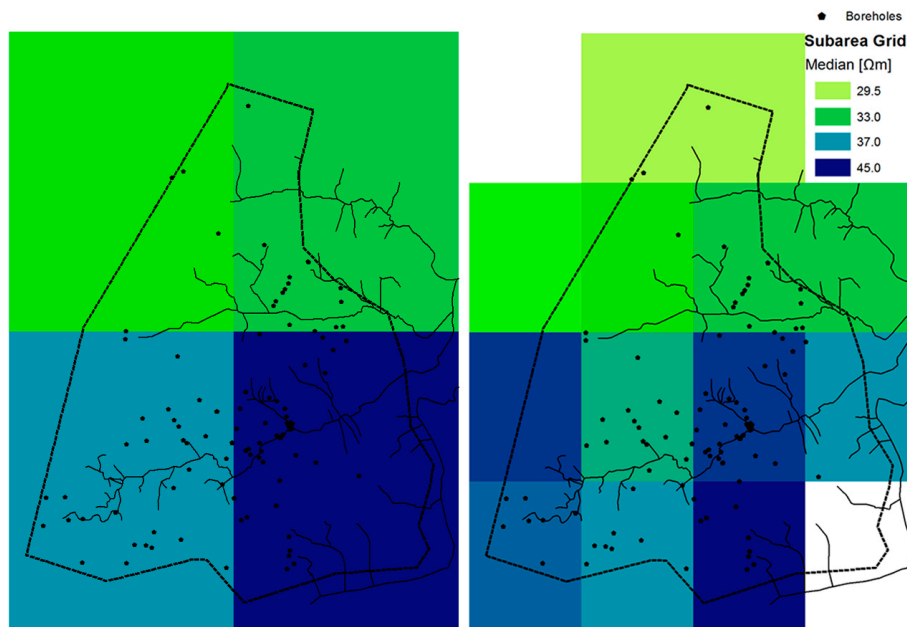
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**Fig. 2.** The median resistivity values from the SkyTEM data for the 4- and 16-subarea grid. Dark colors indicate a high median (max: 43.2 and 45.0  $\Omega\text{m}$  for the 4- and 16-subarea grid, respectively), light colors a low median (min: 32.0 and 29.5  $\Omega\text{m}$  for the 4- and 16-subarea grid, respectively) and white colors the absence of data. Additionally the location of the boreholes, the river network and the delineated glacial structure. The extent is 9 km in  $X$  and 12 km in  $Y$  direction.

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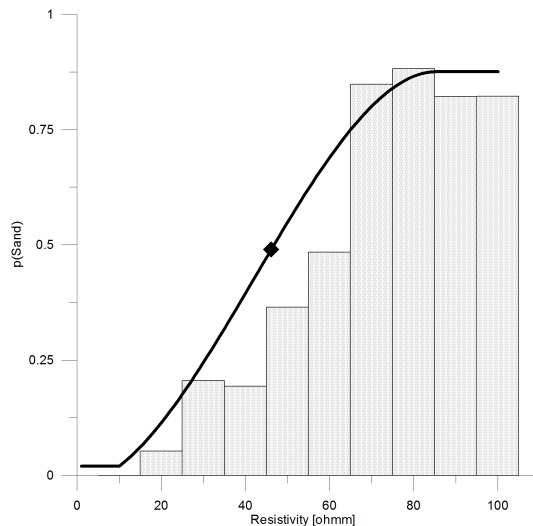
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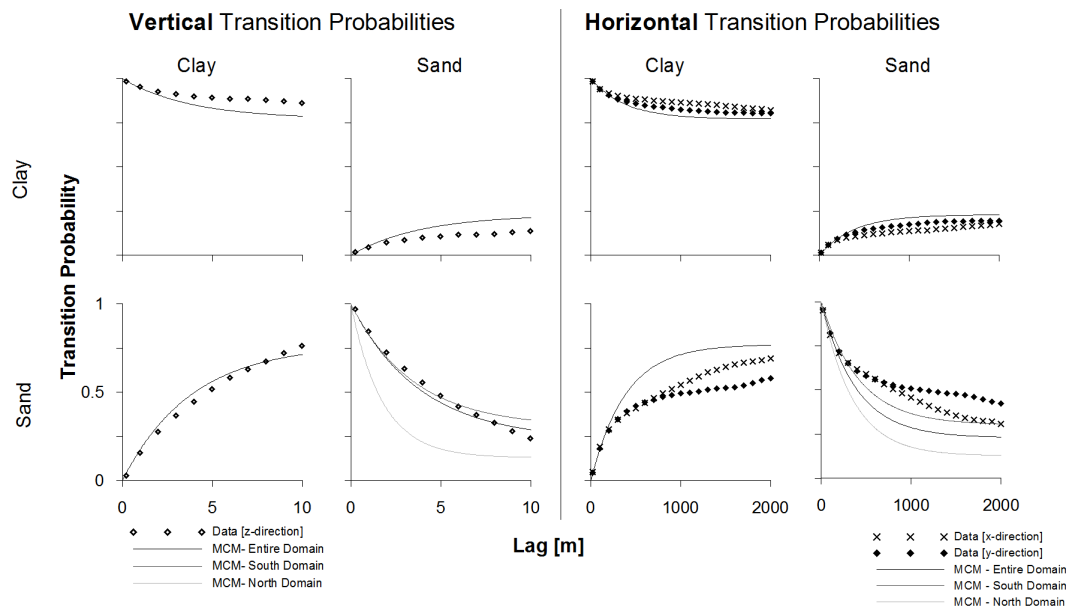
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**Fig. 3.** The bias corrected histogram curve: the calibrated cut off value (46  $\Omega\text{m}$ ) is added to the histogram and the fitted curve is forced to honor it He et al. (2013).

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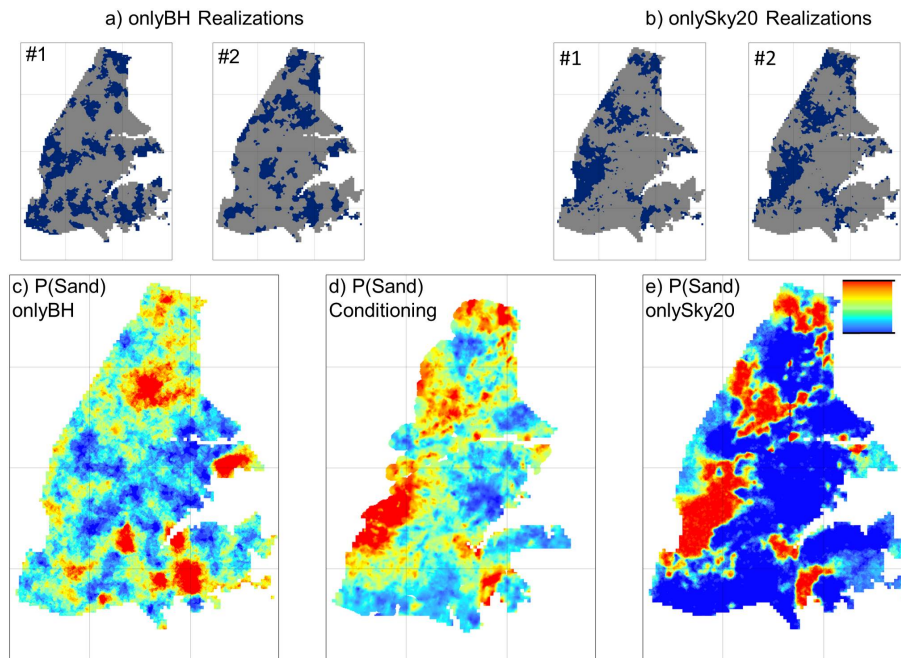


**Fig. 4.** The computed transition probabilities in vertical and horizontal direction and the fitted MCM: vertical 5 m, horizontal 500 m mean length of a sand lens and 23 % sand proportion. Additionally the fitted MCM for the north- and south-sub-domain are plotted for the vertical and horizontal sand-sand transitions: 2 m, 400 m, 13 % and 5 m, 600 m, 30 %, respectively.

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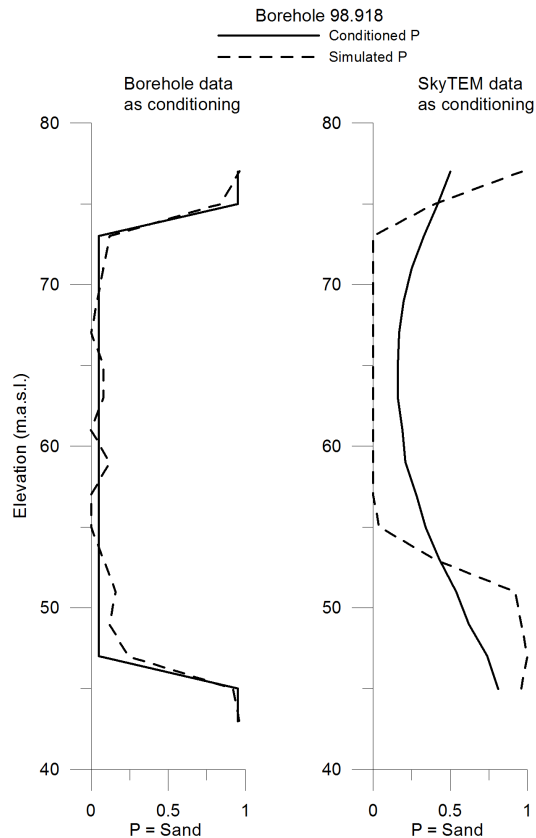
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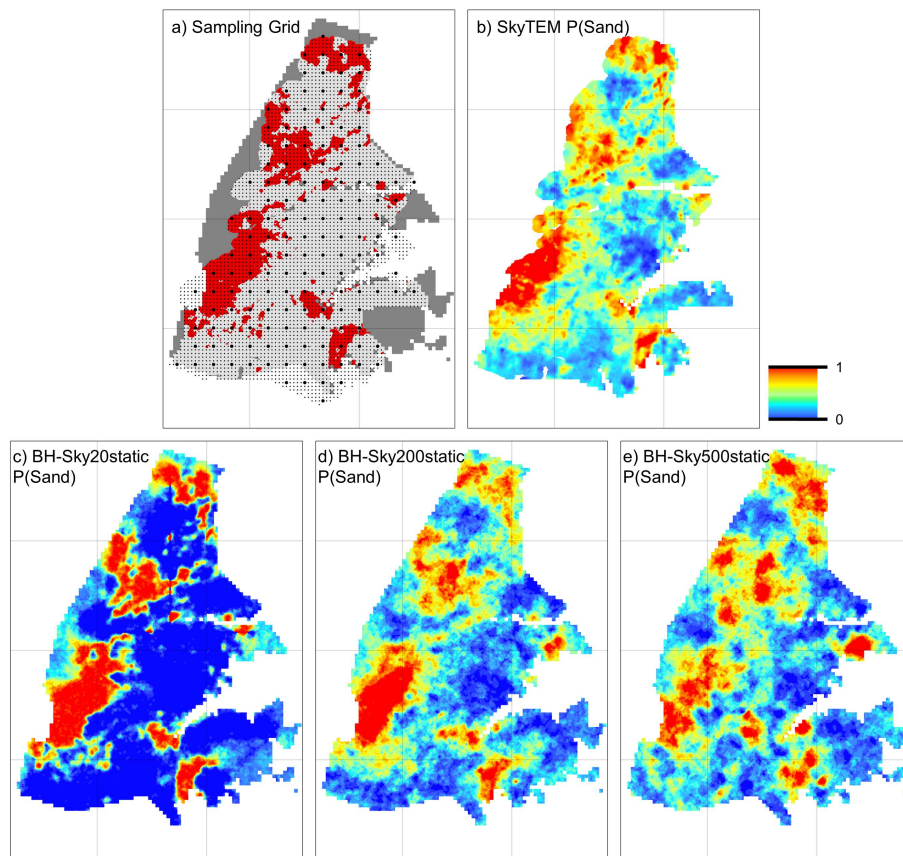


**Fig. 5.** Upper panel: two individual realizations for two different conditioning scenarios: onlyBH (a) and onlySky20 data (b). Lower panel: probability maps for the two scenarios (c) and (e) showing the probability of sand in each cell based on 25 realizations. The derived sand probability which is used for conditioning the simulation is shown in (d). All maps show data at an elevation of 49 m.

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**Fig. 6.** The simulated vs. the conditioned sand probability over the vertical extent at one borehole (98.918), located in the south western part of the glacial structure. The results originate from the two different soft conditioning scenarios: onlyBH and onlySky20 (based on 25 realizations each).

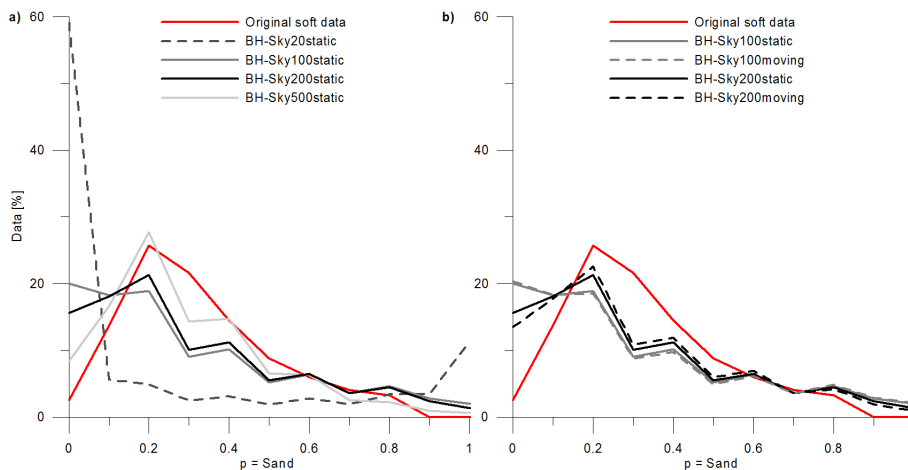


**Fig. 7.** (a) 100 m (small dots) and 500 m (big dots) sampling grids for thinning out the conditioning dataset; (b)–(e) probability of sand at an elevation of 49 m for SkyTEM dataset (b), and for static 20, 200 and 500 m conditioning (c)–(e) red colors represent high sand probability and blue colors low sand probability (based on 25 realizations).



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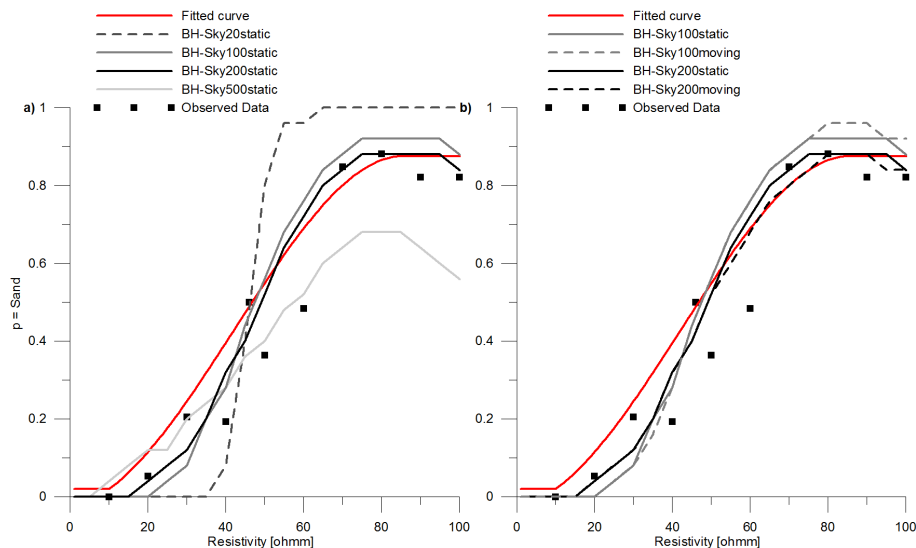


**Fig. 9.** The simulated facies probability distributions based on sets of realizations conditioned to differently sampled soft datasets (based on 25 realizations): **(a)** static sampling at different sampling distances and **(b)** stationary and moving sampling at different sampling distances. Also showing the sand probability distribution of the original soft dataset which is desired to be reproduced.

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**Fig. 10.** The simulated facies probability – resistivity bias based on sets of realizations conditioned to differently sampled soft datasets (based on 25 realizations): **(a)** static sampling at different sampling distances and **(b)** stationary and moving sampling at different sampling distances. The simulated sand probability is paired with the original resistivity value, grouped into  $5\ \Omega\text{m}$  bins and then plotted as median for each bin. Also showing the observed data and the fitted curve from the histogram which is desired to be reproduced.

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