

The Geological Elements approach of MapField:

Detailed mapping and modelling of integrated geological
and redox structures of the subsurface

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1. Foreword

This report is made in the context of the MapField project (www.mapfield.dk) in which scientists, companies, authorities, and the agricultural sector collaborate to develop environmental technologies and methods to be used in future more targeted nitrogen (N) regulation of agriculture. In this context nitrogen, or N, implies reactive nitrogen (nitrate, ammonium, or N in manure) added as fertilizer. The MapField project is highly interdisciplinary and brings together researchers working in areas of geophysics, geology, hydrology, geochemistry, agriculture, and business sciences. The vision is to generate important knowledge about water flow and natural denitrification in the groundwater zone to be able to protect groundwater, streams, and fjords from nitrogen pollution, while at the same time creating better production conditions for agriculture. MapField focuses on the uppermost 30-50 m of the subsurface. In MapField, detailed estimations of the N retention in the subsurface related to individual fields are based on groundwater modelling of water and nitrogen flow pathways, and the N turnover along the flow path from the individual fields. Therefore, it is important to obtain a high level of detail in the descriptions of the geological structures and redox architectures of the subsurface.

In MapField a concept is developed to form the basis for a precise regulation of the agricultural use and management of nitrogen at field level, where actions and mitigation measures are adapted to the nitrogen turnover in the subsurface related to each field. The concept is described in more detail on the homepage of MapField (<https://eng.mapfield.dk/>). Part of the MapField concept is to model the hydrostratigraphic structures and redox architectures important for water transport and natural denitrification in the subsurface. Modelling the lithological variations is based on MPS (**M**ultiple **P**oint (geo)**S**tatistics) simulations using training images based on accumulated clay thickness combined with clustering as described in Vilhelmsen et al. (2019).

This report presents the concept of co-interpretation of geology and geochemistry using the Geological Elements approach developed as a part of MapField at the Department of Groundwater and Quaternary Geology Mapping at GEUS. As redox conditions are closely related to the geology, an approach handling both modelling of the geological and geochemical architectures have been created for use in the subsequent hydrological modelling of N transport and turnover in the MapField project.

Four small agricultural catchments (the LOOP areas), which are part of the National Monitoring Programme (NOVANA), have been chosen as validation sites in MapField. The LOOP areas are so-called ID15 N regulatory catchments of about 1500 hectares. The study areas are located on the island of Funen and in the northern, central, and southern part of Jutland. The areas represent various types of climates, soils, and agriculture, and they also represent geological conditions commonly found in the uppermost layers of the Danish subsurface. The successions found in the areas encompass primarily Quaternary glacial sediments, but older, predominantly marine Paleogene and Neogene sediments are also represented.

This report contains firstly an introduction to the workflow. After that, a description of the data used is followed by individual sections encompassing the geological mapping and modelling,

and lastly the joint statistical modelling of geology and geochemistry. The last two chapters of the report summarize, conclude, and list suggestions for further development of the concept and for other uses of the concept.

2. Introduction

Mapping the 3D geological architecture and characteristics of the subsurface layers, and thereby gaining an understanding of the way the subsurface is formed, is an important part of the approach described in this report. A thorough understanding of the geological processes and the formation of the individual parts of the sedimentary succession helps setting up a robust 3D framework for geology and redox structures before modelling of water flow and nitrogen transport and turnover in the unsaturated and saturated zones of the subsurface.

Understanding the zones of natural denitrification in the subsurface requires geological mapping and models of the shallow subsurface that provide a sufficient degree of detail of the individual parts of the hydrological and geochemical system.

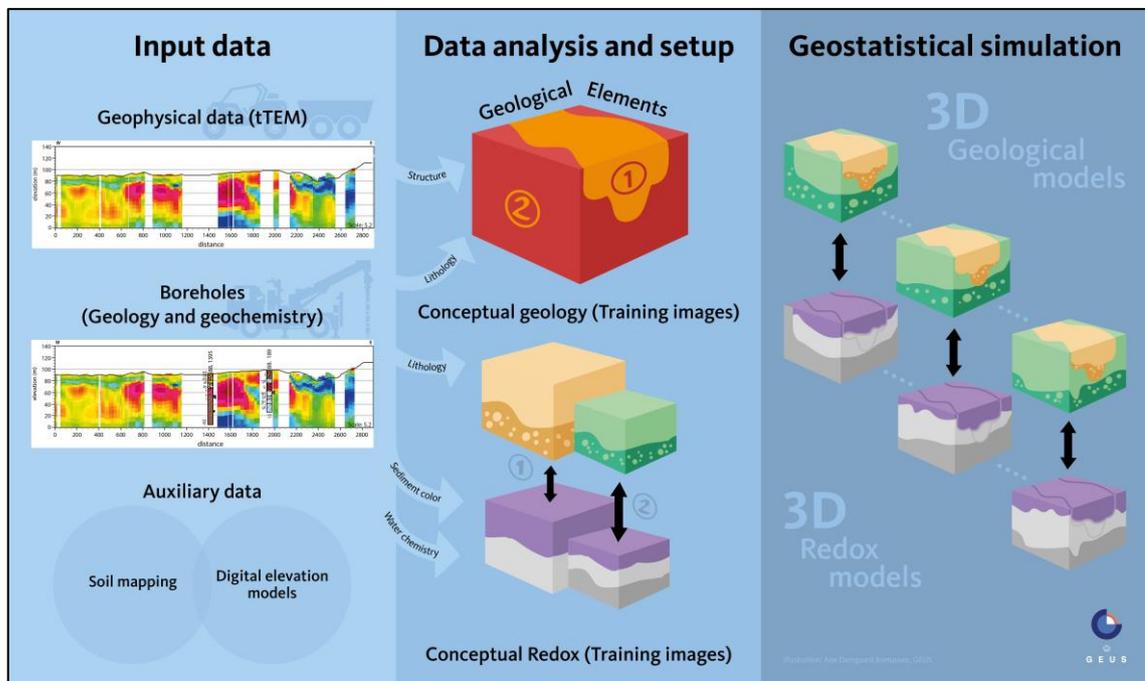


Figure 2-1: A sketch of the general workflow from input data to data analysis, delineating geological elements, and creating Training Images (TI) of geology and redox conditions, before setting up and running geostatistical simulations. From Madsen et al. (2021a).

Figure 2-1 shows a sketch of the overall workflow that has been used for the 3D geological and redox structure modelling and the subsequent geostatistical simulations in MapField. Firstly, input data of different types are collected (left side of the figure) and thereafter, the geology is modelled as Geological Elements (GE), and Training Images (TI) of the conceptual geology and the redox conditions (centre of the figure). Lastly, geostatistical simulations create combined 3D geological and redox models by using Multiple Point (geo)Statistics (MPS) (right side of the figure). The output from the geostatistical simulations is intended for use in hydrological and N transport modelling and lastly for production of N retention maps.

As it is described later in more detail, GEs are defined as ‘*separate volumes of the subsurface representing groups of layers that can be related to specific parts of the geological history of*

the area'. GEs are used to minimise the 3D geological modelling and to generate a simplified subsurface framework for use in the subsequent geostatistical simulations. TIs are made in selected subareas as 3D voxel models which represent the individual GEs as a spatial picture of the structure, lithology, and redox conditions of the GE. Using geological and redox TIs as input for geostatistical modelling is an approach which faces different challenges, such as choosing a representative size of the TI, making it large enough to describe the geological variability. The TI can be constructed from data and models, or through a more arbitrary approach. Descriptions of both GEs and TIs and their use in the concept can be found in more detail in the following chapters.

The Geological Elements approach provides an efficient way of representing highly complex lithological variations without having to generate fully manual and highly detailed 3D geological models, but instead using TIs in combination with statistical modelling in the MapField workflow.

3. Detailed workflow description

The overall workflow shown in Figure 2-1 is simplified, and looking closer, the workflow can be split into a number of tasks where many of these are mutually dependent. This more detailed workflow is shown in Figure 3-1.

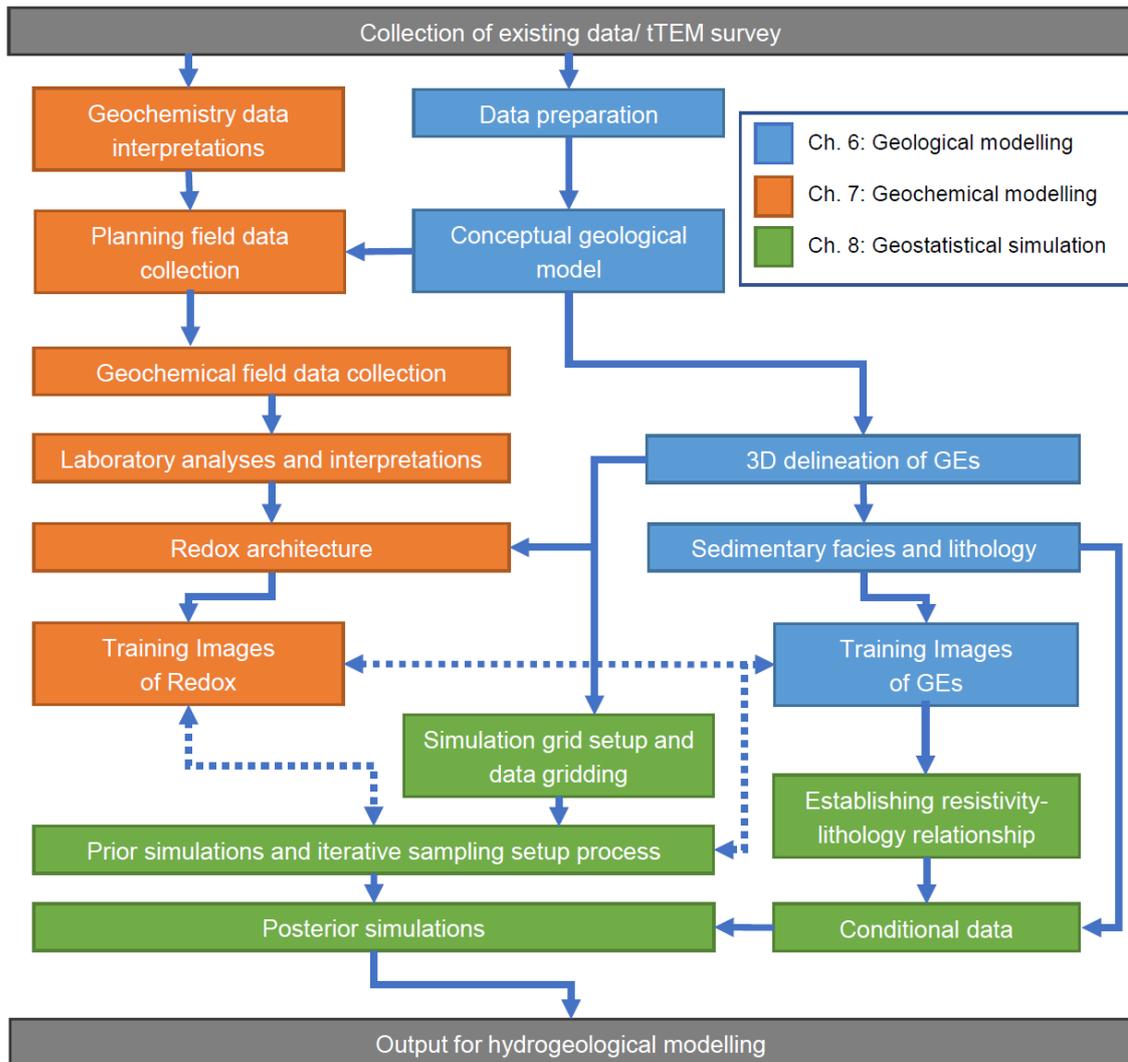


Figure 3-1: Concept workflow. Solid arrows represent exchange of information, data, or interpretations, while dotted arrows represent feedback loops.

In the Geological Elements approach, we combine geological modelling, geochemical interpretation/modelling, and geostatistical simulation, and therefore many of the workflow tasks require exchange of information, data, or interpretations between modellers. In addition to this, feedback loops are important throughout the work process for instance between TI builders (geology and geochemistry), and geostatistical modellers to ensure that the stochastic simulations fit the geological understanding. In these feedback loops the geologists and geochemists are presented with simulation results from the geostatistical modelling to ensure that the results are in accordance with prior knowledge of geology and geochemistry. If the

simulations are not acceptable, the TI is either altered or the simulation algorithm parameterization adjusted.

The detailed workflow of Figure 3-1 has been color-coded so that the tasks of the geological modelling are shown in blue, the geochemical modelling in orange, and the geostatistical simulations in green. The blue solid arrows represent exchange of information, data or interpretations, and dotted arrows represent feedback loops.

The flow is from the top to the bottom; the first tasks are collection of existing data and performance of a geophysical tTEM field survey (top grey box). After preparation of the geological data and interpretation of the geophysical data, a conceptual geological model is constructed. The preliminary geochemical interpretations aim at planning the field data collection, and benefits from the conceptual geological model as a structural and lithological frame of the subsurface. Field samples are geochemically analysed and interpreted. The conceptual geological model leads to a 3D delineation of GEs, which are then used in interpreting the redox architecture and eventually Redox TIs. Geological TIs are constructed for each GE using lithological and structural information. Based on the GEs, the TIs, and the geological and geophysical data, statistical simulations are hereafter performed in a series of feedback loops (as explained above) that end up with simulation outputs in 3D that can be used for subsequent hydrological modelling (bottom grey box).

The individual tasks shown in Figure 3-1 are described in more detail in Chapters 6 to 8.

4. The ‘Geological Elements’ approach

4.1 Geological Elements

The geology of a given part of the subsurface may be simple or complex depending on the geological history and on the depth and the scale at which we observe. Mapping the protection of surface waters demands focus on the upper groundwater (app. 30 meter) while mapping of groundwater resources and their vulnerability normally reaches down to app. 200-300 meters. To model the groundwater flow and model the geochemical processes in the upper 30 meters, it is required to have a geological model that to a high level of detail contains individual layers and their lithology as well as the overall architecture. However, the model detail needed will not be easy to represent using a traditional “layer-cake” model, because of the difficulty in separating and correlating multiple layers - especially in areas with complex geological settings (e.g. Jørgensen et al. 2013).

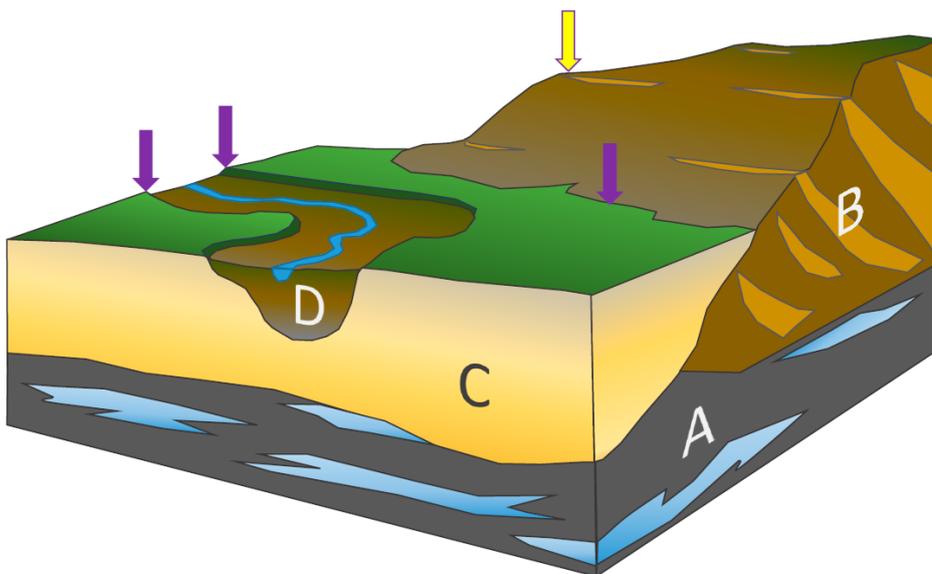


Figure 4-1: An example of well-defined Geological Elements: A) Marine sediments of sand and clay deposited in an offshore environment, B) Glacial sediments of clay till with inclined sand layers, C) Meltwater sediments of sand and gravel deposited on an outwash plain, D) Riverbed sediments of clayey sand with high organic content. Purple and yellow arrows mark topographic indicators (see text).

To overcome this well-known obstacle, we introduce a combination of cognitive modelling of fewer and larger volumes of the subsurface, with geostatistical modelling of the lithology within these individual elements based on geological and geophysical data. We name these subsurface volumes ‘Geological Elements’. The GEs are defined as separate volumes of the subsurface representing groups of layers that can be related to specific parts of the geological history of the area, thus having separate formation histories. The delineation of the subsurface into separate GEs have the advantage that it is only necessary to model the upper and the lower boundaries of a GE consisting of multiple individual layers. The layers between

the upper and lower boundaries of each GE can then be handled and modelled using geo-statistical modelling with Training Images. In this way, we combine manual and semi-automatic modelling procedures performed on well-defined groups of layers in the subsurface. The approach is a further elaboration of concepts described in He et al. (2015), Jørgensen et al. (2015), and Høyer et al. (2015; 2017).

Using the Geological Elements approach, focus is on mapping the architecture of the subsurface as larger, discrete lithological volumes that can be related to distinct parts of the geological history of the area. The understanding of the origin of the GEs makes it possible to construct models that divide the subsurface into a limited number of geologically unique volumes that are separated both physically and chronologically in terms of formation. In addition to the GE boundaries, the geological and geophysical data provide details on the lithological variations within each GE.

Geological Elements (GE)

'The GEs are defined as separate volumes of the subsurface representing groups of layers that can be related to specific parts of the geological history of the area, thus having separate formation histories'.

Modelling fewer geological boundaries and introducing semi-automatic modelling procedures will inevitably lower the amount of time needed for 3D geological modelling. At the same time, it opens for a segmentation of the modelling workflow into well-defined consecutive tasks that can be used in any selected area. The approach also opens for a more straightforward handling of model uncertainties because these can be related to the layer-boundaries and the lithology within the GE separately (e.g., Madsen et al. 2021b). Additionally, the approach most likely makes the dissemination of the subsurface characteristics to stakeholders more intuitive.

Delineating the Geological Elements is an important part of the modelling workflow, where the subsurface of the given area is separated into a small number of GEs – typically 3 to 5. The individual GEs should represent a well-defined part of both the subsurface and the geological history that can be separated from other GEs below and above. In other words, the individual GEs are the result of a certain succession of geological events not shared with the other GEs.

The 3D sketch in Figure 4-1 shows an example where a division into four GEs has been made. The four elements from A to D represent parts of the geological history that have resulted in deposition, whereas the boundaries between them may represent long intervals of erosion or lack of sedimentation. The element A consists of clay with intervening sand layers deposited in a marine environment at some distance from the coast. The sediments show a characteristic distribution of sand lenses. Element B is a body of clay till with an array of inclined sand layers caused by deformation by an advancing ice sheet, whereas element C is an apparently more homogeneous body of sand and gravel deposited on an outwash plain in front of a glacier. Element D is a body of clayey and sandy riverbed sediments with high organic content. The sediments of element D fill an eroded volume of the outwash plain.

The four geological elements are different in many ways: origin, age, boundaries, complexity, lithology etc. The boundaries between the elements are in this example distinct and can

therefore easily be separated. Mapping of the elements can be done using borehole data combined with data from geophysical surveys and information from the topography. As indicated on Figure 4-1, the boundaries between the geological elements can partially be deduced from the topography (purple arrows) and even indications of the internal structure can sometimes be found in the terrain (yellow arrows).

Once the elements have been outlined and separated, the internal structure and lithology of each element can be described based on the available data combined with geological knowledge of the specific type of depositional environment. The boundaries, the internal structure and the lithology of the elements can be mapped and modelled to the desired scale.

However, a successful mapping depends not only on the ability of the used methods to resolve the geological elements, but also on the data density and the data quality. It is therefore important to include an assessment of the uncertainties involved. The uncertainties involved in the mapping relates to the used mapping methods, the data and data processing, the needed degree of detail (scale) and the degree of geological complexity. The uncertainties involved in the construction of the spatial geological model relates to the co-interpretation of the data to delineate architecture, structure, and lithological variations. Added to this, of course, are the uncertainties related to the more technical aspects of the chosen modelling methods such as uncertainties connected to interpolation of surfaces and the variables related to the used statistical methods.

4.2 Geological Elements and Redox Architecture

Different geological elements will show different redox architectures. The evolution of redox architecture is governed by 1) pathways of oxidants (i.e., oxygen and nitrate) delivered via water and gas; 2) availability of electron donors (i.e., organic matter, or Fe(II)-bearing minerals such as pyrite); and 3) cumulative exposure time to oxidation reactions. The geological elements, which are defined by different ages, origins, complexity, and lithologies, will display distinctive characteristics of these three factors shaping the redox architecture. Consequently, the redox architectures will be different for each geological element.

For instance, GE 'C' (the meltwater sediments) in Figure 4-1 may display a planar redox architecture (Figure 4-2a) because of the homogenous hydrogeological structure, vertical infiltration of oxidants (i.e., oxygen and nitrate) via water or gas diffusion may be the dominant pathway (Kim et al., 2019). In addition, due to the homogeneous structure, the availability of the electron donors and the exposure time to oxidation reactions would likely be homogeneous throughout the geological element, resulting in the planar redox architecture type. Compared to this, the GE 'B' will display a more complex redox architecture because of the thrust clay layers (Figure 4-2c). Oxic zones may only develop along the sand zones sandwiched between the thrust clay layers (Kim et al., 2019). Under geologically complex settings, discontinuity of the less permeable layers (i.e., clay) create 'geological windows', which act as pathways delivering oxidants into the deeper subsurface, resulting in highly localized oxic zones (Figure 4.2b).

These conceptual models of redox architecture will be quantitatively expressed by synthesizing geochemical data and geological models. The geochemical observations such as sediment colours, the chemistry of water and sediment will provide information of the depth and extent of different redox conditions. The spatial representativeness, density and quality of the geochemical data will be critical in order to reduce the uncertainty of the geochemical model. Field campaign design based on a prior knowledge of the hydrogeological structure of the subsurface will therefore be greatly beneficial to increase the representativeness of the geochemical data.

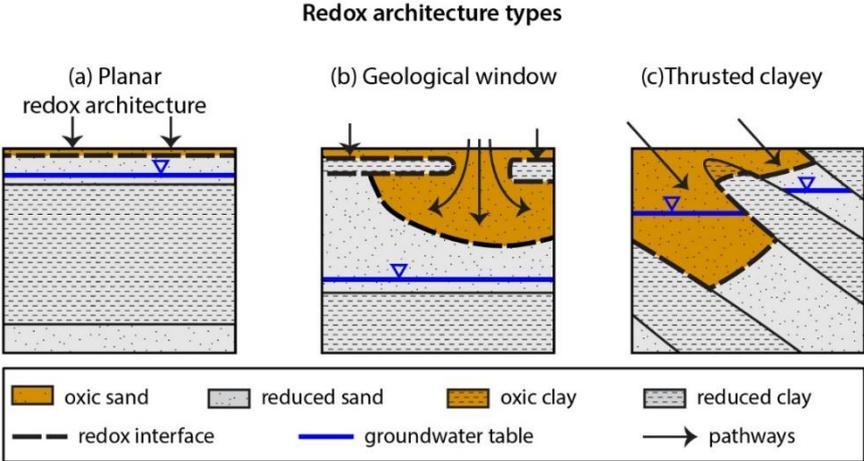


Figure 4-2. Conceptual models of redox architecture types (Kim et al., 2019).

5. Data

5.1 Existing data

Existing geophysical, geological, hydrological, and geochemical data are collected from databases. Because the MapField study areas are often small (app. 1500 hectares) and the amount of existing data often scarce, it is typically required to gather information from surrounding areas.

Existing data used for modelling is shown in Table 5.1. There are basically four types of numerical data: 1) geophysical, 2) geological, 3) geochemical, and 4) hydrological data which are all freely accessible for download through web services. In addition to these digital data, there is also a wealth of reports and other types of publications available as scanned documents in public libraries or in GEUS' report database.

Table 5.1: Overview of types and sources of existing data

Type of data	Data/information	Source
Geophysics	Existing geophysical data	Gerda database (www.geus.dk)
Geology	Borehole data	Jupiter database (www.geus.dk)
	Surface geology map	GEUS maps (www.geus.dk)
	Digital elevation models (DEM)	Datafordeler.dk
	Orthophotographs	Datafordeler.dk
Hydrology	Groundwater table	Jupiter database (www.geus.dk)
	Stream discharge	ODA (https://odaforalle.au.dk/login.aspx)
Geochemistry	Sediment colours	Jupiter database (www.geus.dk)
	Groundwater chemistry (NO ₃ ⁻ , SO ₄ ²⁻ , O ₂ if available)	Jupiter database (www.geus.dk)
	Stream chemistry (NO ₃ ⁻)	ODA (https://odaforalle.au.dk/login.aspx)
General information	Reports and other publications	GEUS Report database/other sources

5.2 Collecting new data

A targeted collection of new data is an important part of the MapField concept and is performed in two campaigns:

1) *t*TEM survey:

A towed-Transient ElectroMagnetic survey (*t*TEM) is chosen as standard because of its ability to map the subsurface resistivity variations with a high degree of detail and with a good data coverage (Auken et al. 2019; Sandersen et al. 2021). The *t*TEM is performed within the study area on all accessible fields.

2) *Detailed geochemical survey*

A field campaign for detailed geochemical investigation is designed based on the preliminary analysis of the subsurface geological and hydrogeological structures using tTEM, background knowledge and relevant data (i.e., groundwater chemistry, groundwater levels). The main objectives of the field campaign are 1) to obtain detailed information about the redox conditions and nitrate propagation of the subsurface; 2) to investigate geochemical conditions of different geological conditions of the subsurface; and 3) to determine denitrification rates of the different geological elements and layers in the subsurface. The selection of the sampling points is based on the availability of the tTEM data, accessibility of the drilling rig and possibilities for reaching the saturated zone of the geological element. During the drilling, core samples are collected.

The samples collected during the field campaigns are analysed for water and sediment chemistry and denitrification rates, and for description of lithology in the laboratories at GEUS. Detailed descriptions of the methods of the chemical analyses of water and sediments are found in the MapField data report (Hansen et al., 2021; Kim et al., 2021b). Briefly, the water samples are analysed for major cations, major anions, ammonium, stable water isotopes, and dissolved organic carbon if the sample volume is large enough. The sediment samples are analysed for the weak acid extractable phase (pH 3 using formic acid) of iron (Fe(II) and Fe(total)). The denitrification rates of the sediment samples were determined using the acetylene-blockage method in batches (Yosinari et al., 1976) in order to enable the analysis of a large number of samples. However other methods such as “push-pull” tests (Kruisdijk and van Breukelen, 2021) could be used.

6. The geological modelling

The geological modelling integrates new as well as existing data and knowledge, and the workflow makes use of newly developed geophysical methods, cognitive-based geological interpretation of the geophysical and geological data and incorporates new high-resolution digital elevation models.

The geological modelling workflow consists of the following steps:

6.1 Data preparation

a) Assessment of existing data

An important part of the planning phase is to assess the existing data in terms of type, age, and coverage. Typically, the existing data in a selected area will comprise borehole data and, in some areas, geophysical data as well. Many datasets can be old and not particularly useful for instance if the coverage is poor or the used methods were less sophisticated, and therefore a careful prioritization of the available existing data is needed.

b) Data preparation

In this step, the geophysical and geological data will be evaluated to identify bad data and perhaps re-interpret existing data. The preparation step has the overall purpose of ensuring that the datasets are optimized for further use and that the uncertainties related to each dataset are assessed and minimized.

The uncertainties related to the construction of geological models are introduced during data collection, data processing, and during the geological interpretations. A thorough assessment of uncertainties involved is complex because both qualitative, semi-quantitative and quantitative uncertainties are involved. At this stage, the quality and uncertainty of the datasets are qualitatively assessed, and faulty data may be removed.

c) Setting up the 3D modelling workspace

The processed data are transferred to the GeoScene3D software (www.l-gis.dk) which is used for the 3D geological modelling process in MapField. GeoScene3D is designed to handle Danish geological and geophysical data from the national borehole database Jupiter and the hydro-geophysical database Gerda (Hansen & Pjetursson, 2011).

All existing and new geological and geophysical data are imported directly into the software (Figure 6-1). Borehole data is accessed through a fully updated Geocloud server containing borehole data, including the new drillings performed as a part of MapField. One or more 3D grids are generated from the geophysical data to serve as support during the geological interpretations and the process of delineating the GEs. The tTEM datasets from the four LOOP areas have a dense data coverage (see Sandersen & Kallesøe, 2021b), and therefore it is possible to perform 3D interpolation with voxel dimensions of e.g. 20 x 20 x 2 m or even 15 x 15 x 1 m.

With the gained overview of the regional geology and the expected geology within the LOOP areas, the scale at which to model the geology can be chosen. Interpretation profiles are typically laid out in a network that crosses important data and at the same time cross anticipated geological structures. A modelling space including all datasets, a database with interpretation points, 2D and 3D grids, is then set up. More information on the GeoScene3D software can be found at www.i-gis.dk, and more information on typical procedures for 3D geological modelling in Denmark can be found in Sandersen et al. (2018) or at https://www.geo-vejledning.dk/2018_1/indhold/ (in Danish).

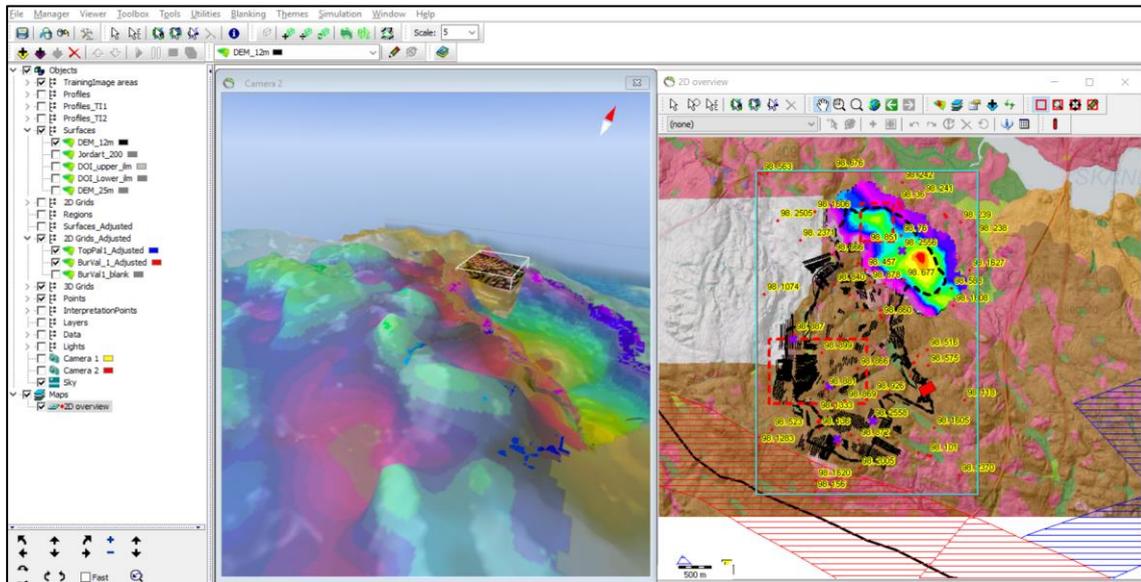


Figure 6-1. Screenshot from the modelling space in GeoScene3D. An example from LOOP 3, Ejer Bavnehøj.

6.2 Constructing a conceptual geological model

In the next step, the construction of the 3D geological model focuses on delineation of the spatial outline of GEs, establishing an event chronology, performing a description of facies and lithology variations of the individual GEs, and finally producing TIs. This process is described in the following:

Data inside and outside the study area are interpreted with the purpose of establishing a conceptual model of the geology. Joint interpretations of the datasets are performed on cross-sections in GeoScene3D, and major layer boundaries are sketched (Figure 6-2).

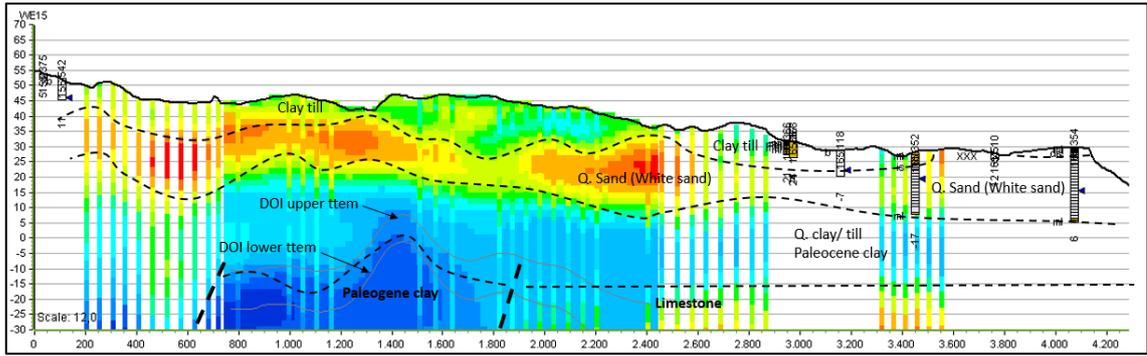
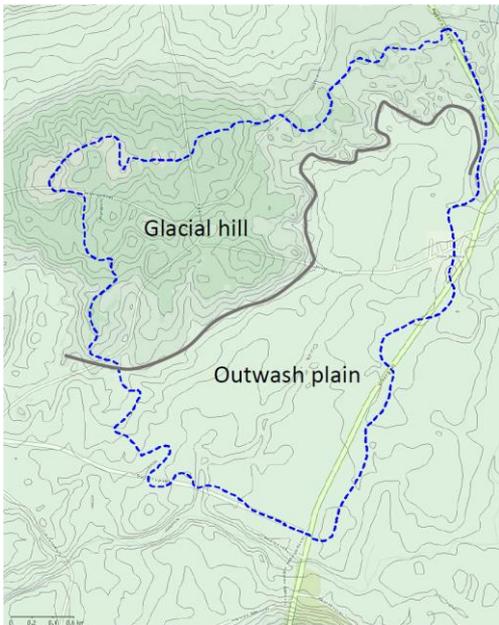


Figure 6-2: An example of geological interpretations along a cross-section from LOOP 4 (Sandersen & Kallesøe, 2021b). tTEM data are shown as a section through the 3D resistivity grid and SkyTEM data are visualized as single soundings. Boreholes are shown as, vertical, sectioned rectangles.



Digital elevation models of the study area form the basis for a delineation of areas with different topography and designating these to specific landforms (Figure 6-3). In addition to this, other features of the landscape, such as stream beds, slope changes, hill orientation, surface lineation, erosional features etc. are described. The interpretation of the topography is then combined with surface geology maps showing the interpreted geology at 1 m depth (Figure 6-4), and a sketch of geological elements is made.

Figure 6-3: Landforms inside the LOOP 2 area (blue hatched line) delineated from the topography. Grey line marks the boundary between the glacial hills and the outwash plain. See Sandersen & Kallesøe (2021a,b).

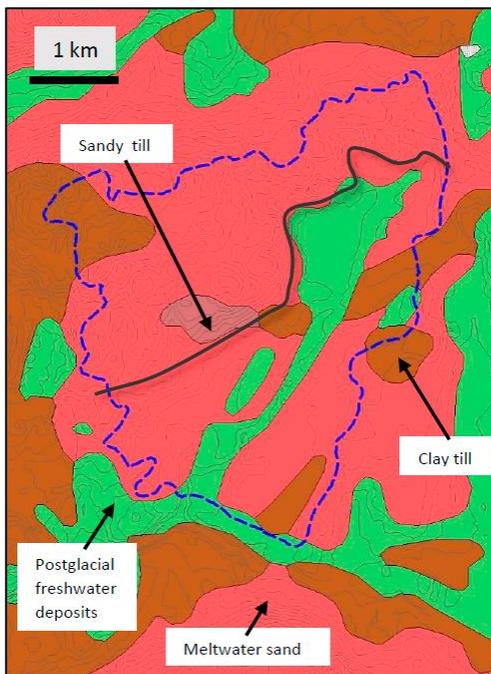


Figure 6-4: Surface geology of the uppermost meter in LOOP 2 (Jakobsen & Tougaard, 2020). Grey line marks the boundary between the glacial hills and the outwash plain.

6.3 3D delineation of GEs

After the conceptualisation of the subsurface, a separation into GEs with a unique formation history are sketched. Interpretations of top and bottom surfaces of the GEs along profiles are performed (point interpretations). As the GEs share tops or bottoms, the output is typically a limited number of GE bottom surfaces.

Delineating the specific GEs is done by surface modelling of the element boundaries. In practice this is done by inserting interpretation points in the 3D space, and afterwards performing interpolation of the points on the individual surfaces. This creates grid surfaces of the element boundaries. Each interpolation point comes with an attribute describing if the point is based on interpretation of data or is based on the conceptual understanding of the geology. An example of interpreted boundaries defining the geological elements in LOOP 2 is shown in Figure 6-5.

Delineating geological elements by cognitive 3D modelling includes scientifically motivated subjective decisions based on geological background knowledge in combination with the specific data. An active choice is made when delineating each GE, and in this process, we appoint uncertainty values to each interpretation point defining the bounding surfaces. Doing this, an overall uncertainty evaluation is attached to the boundaries between geological elements, which can be included in the subsequent geostatistical modelling (Madsen et al., 2021a, 2021b). The evaluation of uncertainties related to the delineation of the GEs is therefore limited to a qualitative assessment of the individual interpretation points of the GE surfaces and a semi-quantitative assessment of the GE lithology performed as a part of the stochastic modelling.

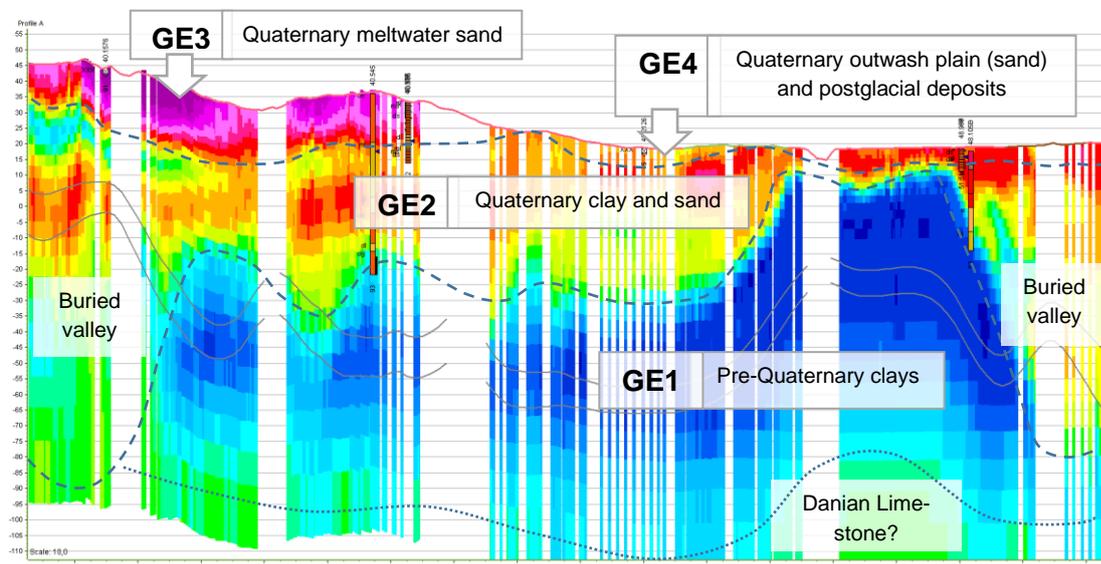


Figure 6-5. Interpreted geological elements GE1 to GE4 shown on a NW-SE profile from LOOP 2. The tTEM resistivity models are shown as coloured vertical lines (blue/green: low resistivities; yellow/red/purple: high resistivities). A few boreholes are shown as sectioned vertical rectangles. From Sandersen & Kallesøe (2021a).

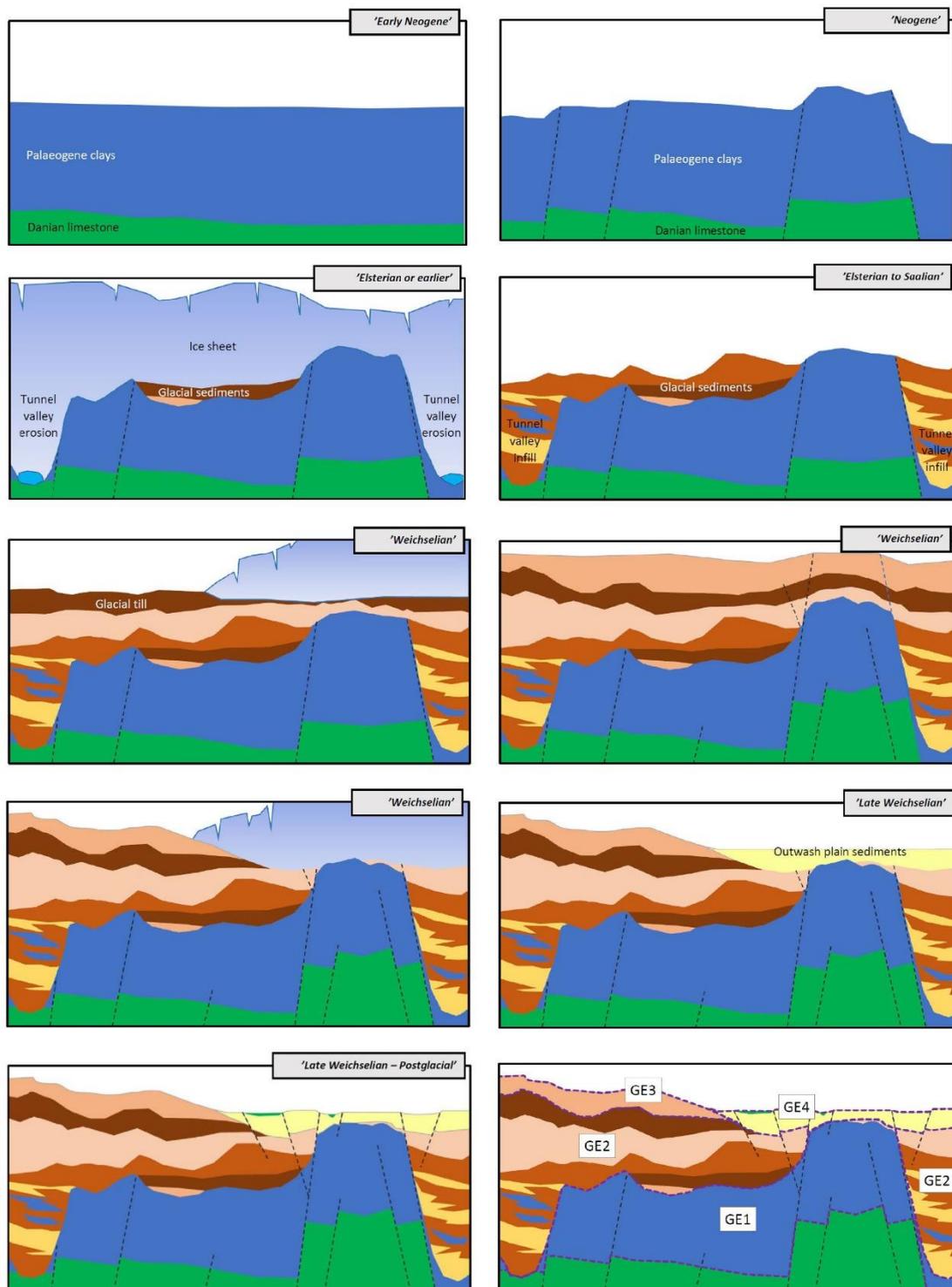


Figure 6-6: Selected Geological Event Chronology sketches from the LOOP 2 area. The sketch in the lower right corner shows the geological elements of LOOP 2 (see Figure 6.5). Adapted from Sandersen & Kallesøe (2021a).

Based on the interpretations described above, a Geological Event Chronology is established. The event chronology aids in understanding the architecture of the layer succession and describes the chain of events responsible for the present appearance of the GEs. The event chronology requires a general knowledge of the geological history of the region around the

study area because significant geological events will most likely have affected the study area even though this cannot be deduced from the local data. Also, information on deep structures may not be available locally, but instead regionally (see Sandersen & Kallesøe 2021a).

The event chronology, when described as sketches as shown in Figure 6-6, is also intended to give stakeholders a better visual understanding of the formation of the subsurface and a better understanding and description of the internal build of the individual geological elements.

6.4 Descriptions of sedimentary facies and lithology

The geological interpretations are finalized with descriptions of facies variations and/or lithological variations to be used for input to the statistical modelling of the lithology inside the individual GEs. The tTEM-data will provide a higher degree of detail than previously obtained with other geophysical methods (Auken et al., 2019; Sandersen et al., 2021) and will therefore – in combination with borehole information - generally provide sufficient detail for descriptions of lithological variations within the GEs.

Each appointed GE can contain several different lithologies with diverse hydraulic properties. Therefore, it is often necessary to establish lithology groups that combine the described lithologies from boreholes and from the surface geology map. Taking LOOP 3 as an example, seven overall lithology groups have been designated (Table 6.1):

Table 6.1: Designated lithology groups in LOOP 3 (see Madsen et al., 2021a).

No.	Group name	Lithology
1	Clay till	ML, (L)
2	Meltwater sand/gravel	DS, DS-DG, DG, G, S, TS, (O)
3	Meltwater clay/silt	DL, DI, DV, (FL)
4	Sandy till	MS, MG
5	Postglacial (partly org.)	FP, FT, FS
6	Pre-Quaternary clay	LL, SL, VL, (GL)
7	Unknown	B, U, X

The GE defining the hydraulically impermeable Paleogene clay in LOOP 3 is simple and contains only one lithology group (6 – Pre-Quaternary Clay), whereas the other two geological elements, a Quaternary succession and buried valley both contain lithology group 1-5. To reduce the number of lithologies within a certain element it is typically necessary to estimate the hydraulic properties and combine sediment types with expected similar properties. Likewise, it is important to choose a reasonable number of classes (variables) having the subsequent stochastic simulations in mind.

6.5 Constructing Training Images (TIs)

Construction of TIs of the individual GEs is based on the geological modelling and on the mapped lithological variations. As mentioned earlier, there are challenges such as choosing a representative size of the TI, so that it is large enough to represent the geological variations.

The TIs are constructed as 3D volumes found to be representative for the individual GEs. Within these volumes, the voxels are interpreted manually, and each voxel is assigned with a lithology class (see Figure 6-7). The construction of the TIs can be done directly, based on the data or through more arbitrary approaches using general knowledge. In MapField we investigate several approaches. The construction of the TIs is entirely done in Geo-Scene3D's voxel module, which ensures that the delineation of voxelated TIs can be visualised together with the modelled GE boundary surfaces and all relevant data.

The intention is to store the TIs in a database opening for either entirely or partly re-use in future project areas with comparable geological elements.

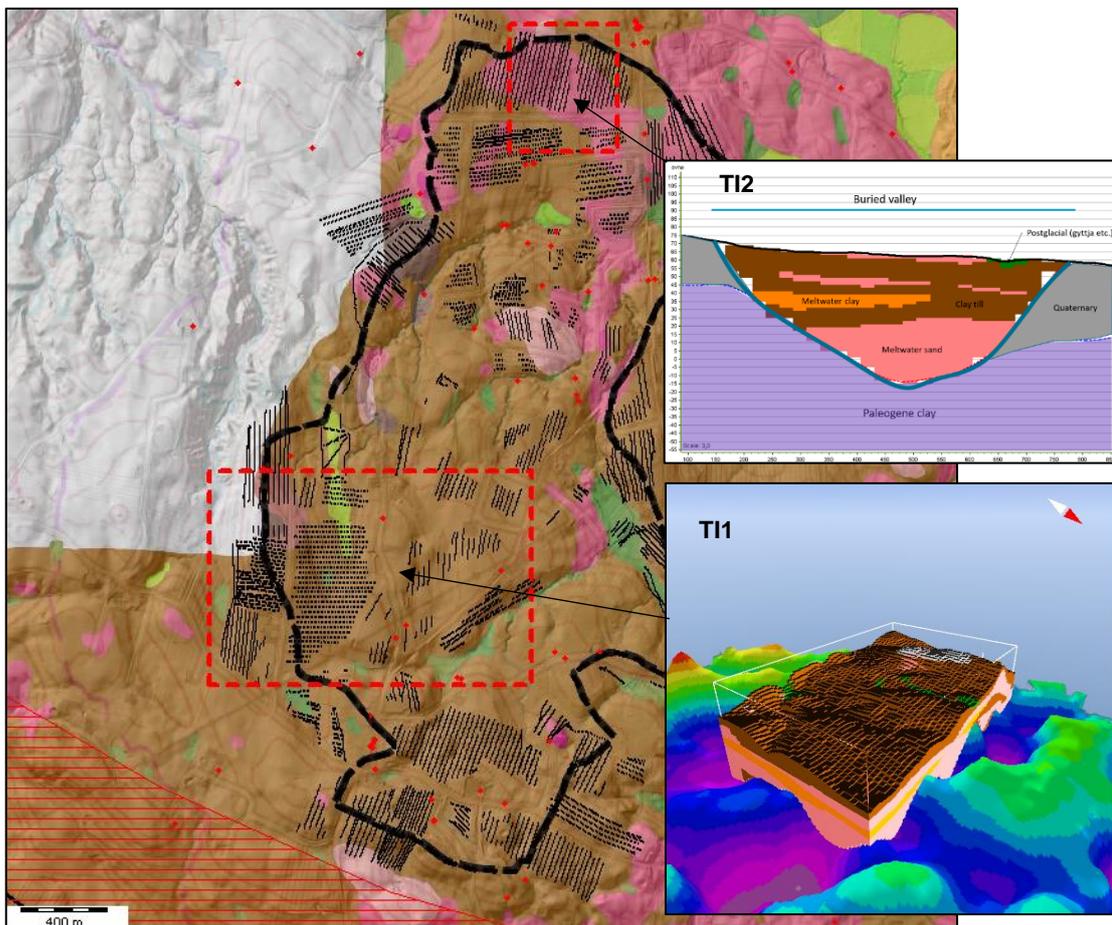


Figure 6-7. An example of TIs from the LOOP 3 area. Both TIs are in 3D; T1 is shown in 3D view and T12 is shown as a 2D cross-section through the TI. See Sandersen & Kalløe (2021b).

Figure 6-7 shows the two selected TI areas of LOOP 3, which are expected to represent the overall geology within the delineated GEs.

7. Geochemical modelling

The geochemical (redox) structure of the subsurface is governed by a complex interplay between geology, hydrology, and biogeochemistry. Therefore, the geochemical modelling requires multi-disciplinary data integration and interpretation. The outcome of this work step is a redox training image for the geostatistical modelling.

7.1 Interpretations of the geochemical data

Redox conditions are interpreted for three different redox zones: 1) oxic conditions where oxygen and nitrate concentrations are high; 2) N-reducing conditions where oxygen is depleted, and nitrate is being reduced; and 3) reduced conditions where nitrate is completely depleted. The redox conditions are defined by three parameters: 1) sediment colours, 2) water chemistry i.e., dissolved oxygen (DO) and nitrate concentrations of groundwater, and 3) sediment chemistry i.e., the Fe(II) to Fe(total) fraction of the sediments (Table 7.1). The redox conditions of all the existing and newly collected data of geochemistry are interpreted based on the criteria described in Table 7.1.

Table 7.1: Criteria for the redox interpretations (Hansen et al., 2021).

Redox condition	Sediment colour*	Water chemistry*	Sediment chemistry**
Oxic	Yellow, orange, red, or combination of these colours	Detectable DO and high nitrate	Weak acid extractable Fe(II)/Fe(total) fraction close to 0
N-reducing	Mixture of oxic and reduced colours (e.g., yellowish grey)	DO free and low nitrate	Weak acid extractable Fe(II)/Fe(total) fraction between 0 and 1
Reduced	Gray, green, blue, black, dark brown or combination of these colours	DO and nitrate free	Weak acid extractable Fe(II)/Fe(total) fraction close to 1

*Mainly existing data (source: Jupiter) but also collected in MapField; **Collected only in MapField

Figure 7-1 shows an example of the results of the detailed geochemical investigation of LOOP3 (Kim et al., 2021b). In LOOP3, the samples were collected at eight locations to represent different hydrogeological characteristics. The redox interpretations based on the criteria described in Table 7.1 are shown in the background as oxic in pink, N-reducing in yellow, and reduced in grey (Figure 7-1).

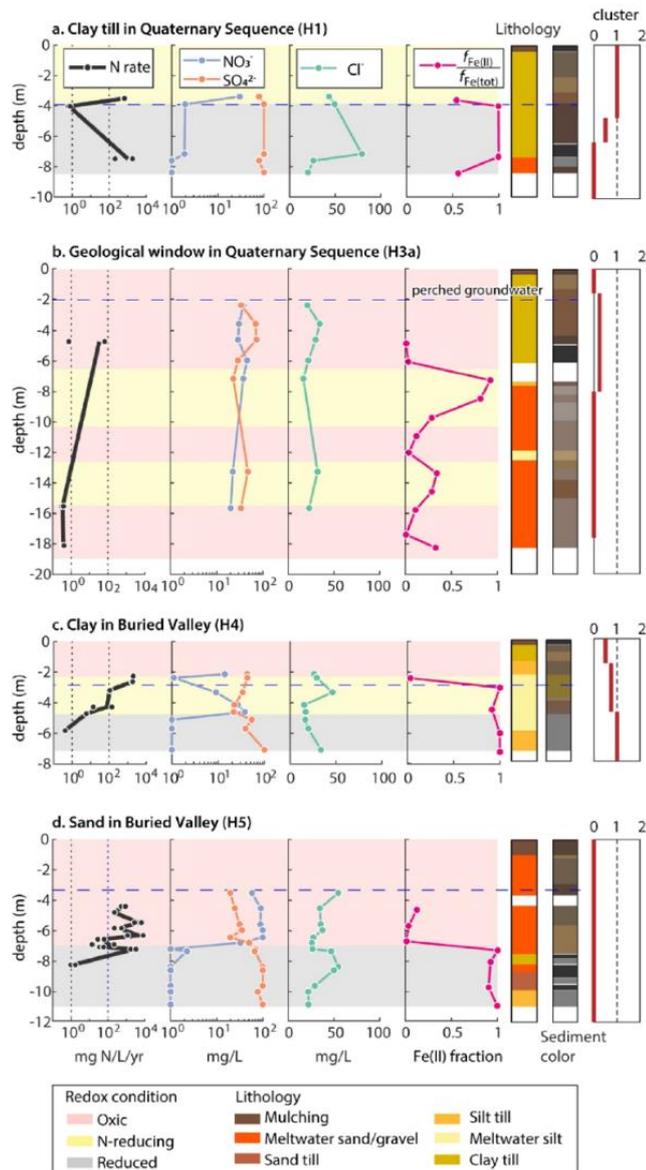


Figure 7-1. Example of results of detailed geochemical investigation in LOOP3. For the redox interpretations, the denitrification rates (1st column), the concentrations of nitrate and sulphate (2nd column), the concentrations of chloride and $\delta^{18}\text{O}$ (3rd column), the Fe(II) to Fe(total) fraction of the weak acid extractable form of the sediment (4th column), lithology (5th column), and the sediment colours (6th column). (Modified Figure 2 in Kim et al. 2021b).

7.2 Conceptual model of the evolution of redox architecture

The geochemical data provide information about the subsurface redox condition at point (i.e., water and sediment chemistry) to 1D (i.e., sediment colour) scales (Figure 7-1). To upscale this information, the results of redox interpretations are further analysed in the context of the geological structure, by overlaying the redox interpretations on the tTEM model and geological interpretations (Figure 7-2)

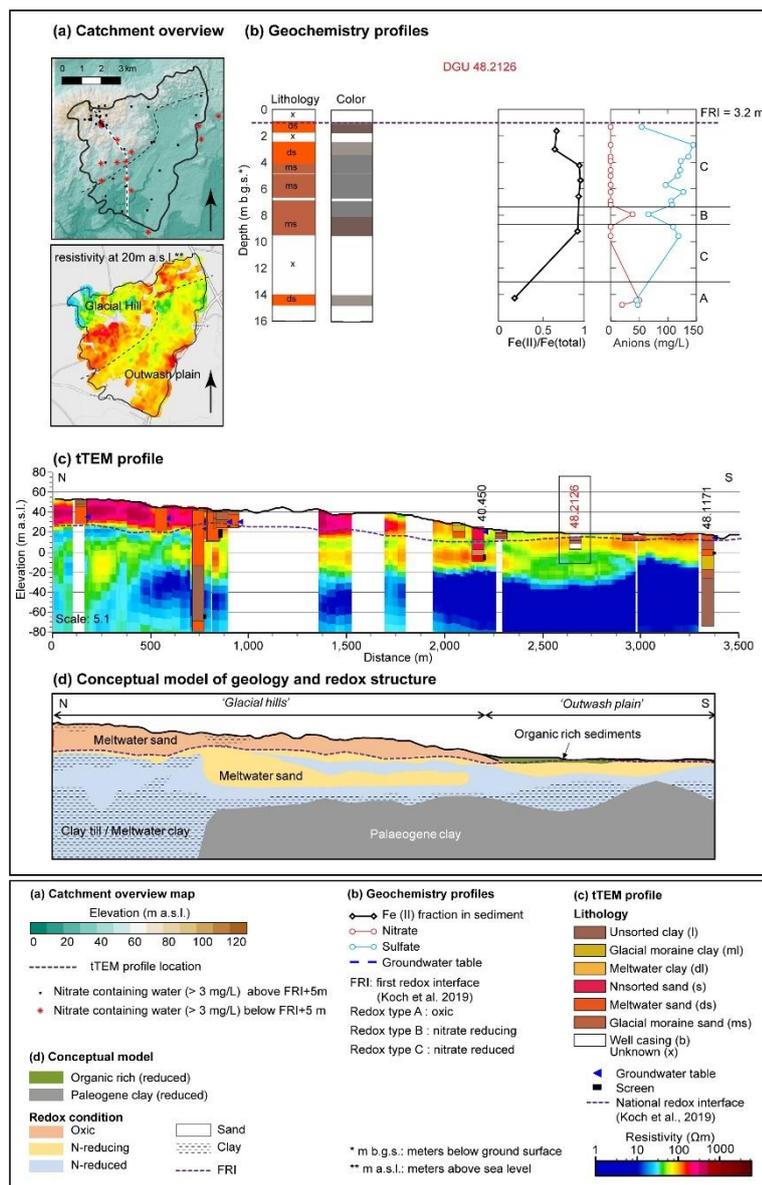


Figure 7-2. Example of redox interpretations of the chemistry of water and sediment and sediment colours in LOOP2. The tTEM profiles and its conceptual interpretations of the geological and redox structures are shown in c and d (Hansen et al., 2021).

The combined conceptual models of geological structures and redox architectures (Figure 7.2.c) are based on mapping of the subsurface structures, and a process-based understanding of the geology and geochemistry. For instance, Kim et al., (2021a) analysed the groundwater chemistry data of LOOP2 and found four discrete groundwater units, where their water chemistries were governed by different hydrogeochemical processes. The locations and governing processes of each groundwater unit can be explained by the geological elements and their weathering/depositional history. The process-based understandings provide a scientific basis for upscaling the point scale information to the catchment scale resulting in a high scientific validity of the geochemical model.

7.3 Converting the Geological TI to Redox TI

By combining the conceptual models of the redox architecture and geochemical data, a set of empirical rules are developed to convert the geological training images to redox training images. The rules define the depth and extent of different redox zones for different lithologies (usually sand and clay) for each geological unit. For instance, in LOOP3, the sand (H3a) in the geological window of the Quaternary sequence (Figure 7-3) showed a thick oxidic layer (>18 meters) and its redox conditions may shift between oxidic and N-reducing conditions multiple times (Figure 7-1). While sand (H5) in the buried valley (Figure 7-3) showed a thin oxidic layer and a simple transition from oxidic to reduced at around 7 meters. These observations imply that the conceptual model of redox architecture of the Quaternary sequence was the geological window type (Figure 4-2b) and the uppermost part of the buried valley was the planar type (Figure 4-2a) (Madsen et al., 2021a).

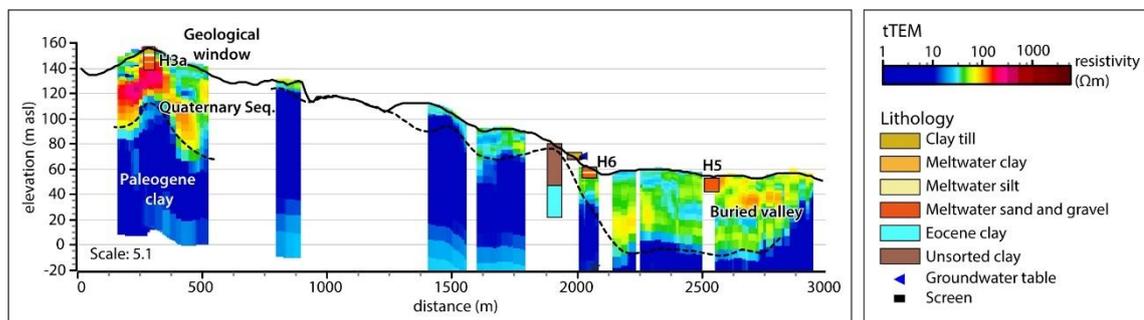


Figure 7-3. tTEM transect of LOOP3 and locations of three boreholes of the detailed geochemical survey. LOOP3 consists of two geological elements: 1) Quaternary Sequence; and 2) Buried valley. In the Quaternary sequence, a large geological window is located at the recharging area. The results of the detailed geochemical investigation of H3a and H5 are shown in Figure 7-1. (Kim et al., 2021b).

Based on the conceptual model of the geological structure and redox architecture, the geochemical data i.e., sediment colours, water and sediment chemistry of each geological element were compiled. The results of redox interpretations of all the geochemical data were discretized into 1-meter intervals and then compiled (i.e., Figure 7-4). An inconsistency between the water/sediment chemistry data and the sediment colour data are sometimes observed. This difference may be because the water/sediment chemistry represent a snapshot of the transient condition of the redox status while the sediment colours may be a cumulative resultant of the oxidation processes over the entire weathering period (Madsen et al., 2021a). This work process aims to build a joint model of geological structure and redox architecture. Thus, to maintain the presumed consistency of the temporal scale between geological structure and redox architecture, the sediment colour results are often prioritized over the water/sediment chemistry data. However, the weighting factor of the different geochemical data should be adjusted depending on for example the quality of the data.

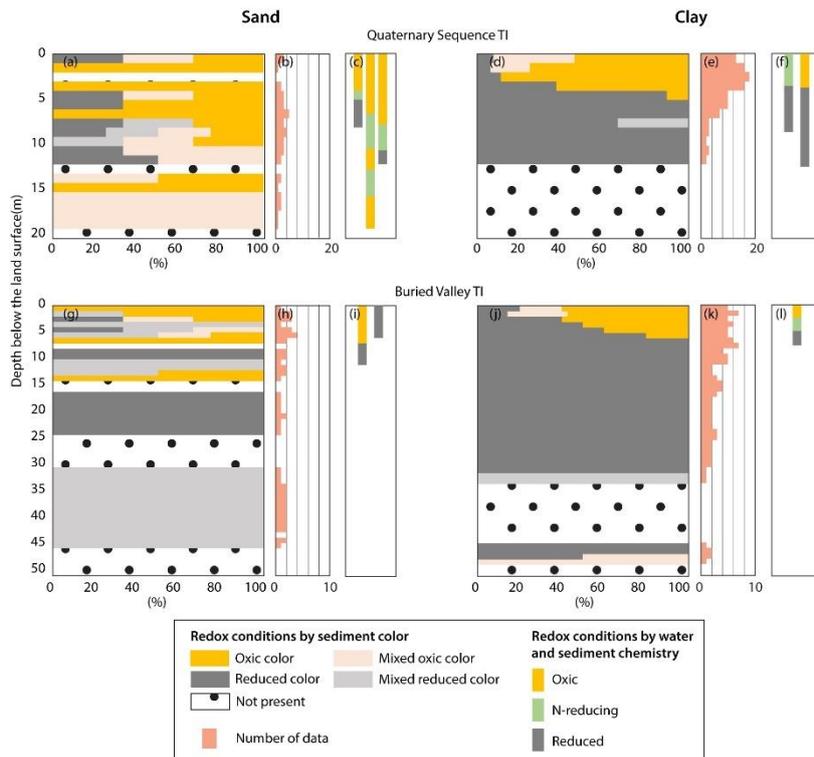


Figure 7-4. Summary of the redox interpretations based on the sediment colours (a, d, g, and j) and the chemistry of water and sediment (c, f, i, and l) of LOOP3. The number of sediment data are shown in b, e, h, and k. The results are shown separately for sand (left) and clay (right) in the Quaternary sequence TI (top) and buried valley (bottom; Figure 5 in Madsen et al., 2021a).

Figure 7-4 shows the results of the data discretization and compilation of LOOP3 as an example (Madsen et al., 2021a). Based on these data, the empirical rules to convert the geological TI to a redox TI are set. In this work process, Matlab was used to convert the TIs. The empirical rules differ from site to site. Here are the conversion rules of LOOP3 defined based on Figure 7-4 (Madsen et al., 2021a):

For sand in the Quaternary sequence TI (TI1):

- 1) For the first layer (0-2 meters), from high to low elevation, 80% of meltwater sand in the geological window is oxidic, 10% of the rest is N reducing condition, and then the rest 10 % is reduced conditions.
- 2) The oxidic voxels in the first layer are oxidic down to 20 m below the land surface (m bls).
- 3) The sand in the geological window, the fraction of oxidic voxels decrease by 10% for every layer (2 meters) in the 20-30 m bls interval and decreases by 20% for every layer (2 meters) deeper than 30 m bls.
- 4) The N-reducing condition voxels are always located at the edges of oxidic conditions, and the maximum fraction of the N-reducing condition voxels is limited to 10 % of the total sandy voxels per layer.
- 5) The rest is reduced condition.

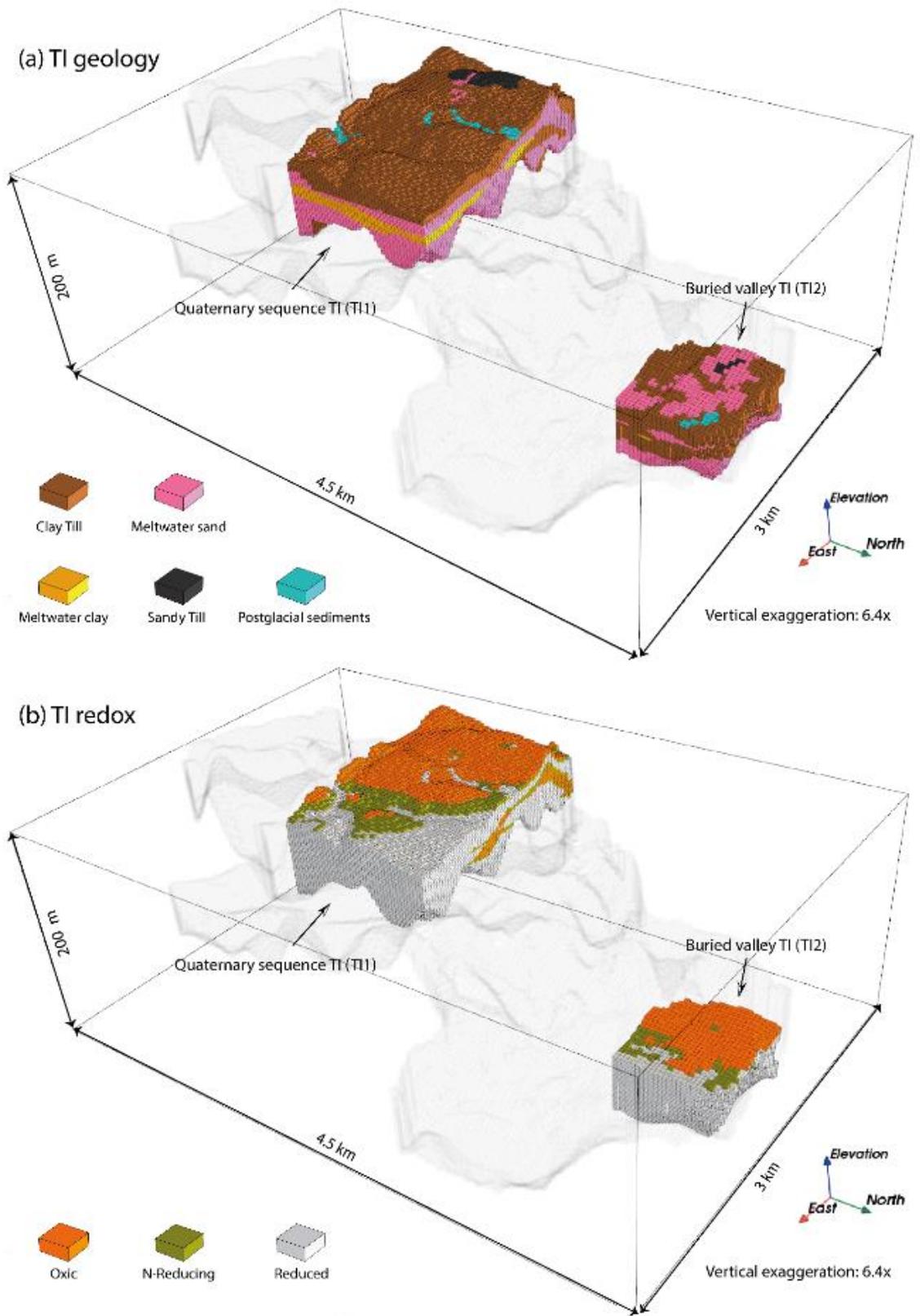


Figure 7-5: TIs for the two GE is LOOP3. a) geological TIs and b) redox TIs. Figure from Madsen et al., 2021a.

For clay (clay till and meltwater clay) in the Quaternary sequence TI (TI1):

- 1) For the first layer (0-2 meters), from high to low elevation, 60%, 20% and 20% of the voxels were oxic, N-reducing, and reduced conditions are distributed.
- 2) With increasing depth down to 6 m bls, for each layer, the fractions of N-reducing and reduced conditions increase by 10% and 20%, respectively, compared to those of the overlying layer.
- 3) Below 6 m bls, clay is always reduced.

For sand in the buried valley (TI2):

- 1) For the first layer (0-2 meters), from high to low elevation, 80%, 10% and 10% of the voxels were oxic, N-reducing, and reduced conditions are distributed.
- 2) With increasing depth, for each layer, the fractions of oxic and N-reducing condition voxels decrease by 70% and 50%, respectively, compared to those of the overlying layer. The rest was reduced.

For clay in the buried valley (TI2):

- 1) For the first layer (0-2 meters), from high to low elevation, 60%, 20% and 20% of the voxels were oxic, N-reducing, and reduced conditions are distributed.
- 2) With increasing depth, for each layer, the fractions of oxic and N-reducing condition voxels decrease by 60% and 20%, respectively, compared to those of the overlying layer. The rest was reduced.

Figure 7.5b shows the final redox TIs for LOOP3 based on the rules described above and the geological TIs shown in Figure 7.5a.

8. Geostatistical simulation

Once the GEs and redox TIs exist, these are used for geostatistical simulation of the catchment area. In the following the modelling steps needed for setting up the geostatistical modelling are presented.

The geostatistical approach used in this project is called MPS and is based on describing the spatial variability of the system in TIs. In contrast to more traditional geostatistical approaches, that rely on spatial relationships between points being described as a function of distance, MPS can simulate using higher-order statistics (Mariethoz and Caers 2015). In practice this means that complex structures and architecture as portrayed in the TIs can be used as a blueprint for simulating similar structures. This naturally leads to more geological/redox realism and connectivity over longer distances than possible through simulations based on the distance between points. Several MPS algorithms are available today that transform the information in the training images to conditional probabilities that can be used when simulated. Here we make use of direct sampling (DS) as this is one of the few algorithms that enables the use of a bivariate TI (Mariethoz et al. 2010). Since the TIs contain coherent information on geology and redox (see section 7.3), they need to be simulated simultaneously and hence the ability to use a bivariate TI is a prerequisite.

8.1 Simulation grid setup and data gridding

First the simulation grid needs to be set up according to the chosen resolution in the geological modelling. Typically, the choice is to use a 25 m x 25 m resolution in the horizontal plane, because hydrological models rarely use finer resolutions in catchment scale modelling. This spacing is also partially determined by the horizontal resolution of the tTEM measurements. Either a 1 m or 2 m spacing is used vertically, depending on the input from the TIs.

The top of the simulation domain is bounded by the terrain from digital elevation models (DEM) that have been scaled to the right horizontal resolution by resampling a high-resolution DEM in the GeoScene3D Toolbox (standalone application). The catchment area is used for bounding the simulation domain in the plane and the bottom is either chosen as a fixed depth or in cases with an impermeable hydraulic boundary, such as Paleogene clay, the lower GE boundary is used. The simulation grid is then split into GEs by the interpreted GE boundaries. Figure 8-1 shows an example of a simulation grid from LOOP3. Three GEs are identified – 1) a Quaternary sequence (pink), 2) a buried valley (green) and a Paleogene clay package. The Paleogene clay is used as the lower boundary for the simulation grid in Figure 8-1b while the GE boundaries are used to delineate the GEs within the simulation grid. This grid has the resolution 25 m x 25 m x 2 m.

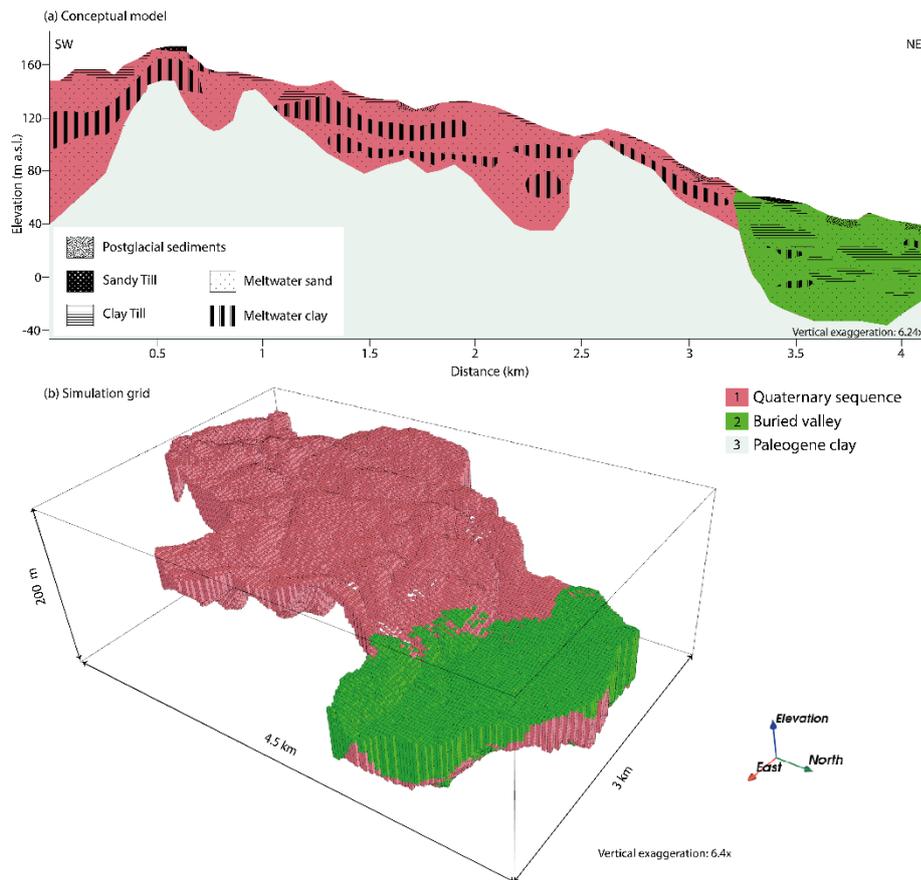


Figure 8-1: Example of simulation grid from LOOP3 from Madsen et al., 2021a. a) a conceptual model of the subsurface divided into three GEs. b) the simulation grid at 25 m x 25 m x 2 m resolution.

The available data are gridded to match the simulation grid. Sometimes more than one tTEM sounding is present within a grid cell, and if this is the case, the sounding nearest to the grid cell centre is used. Alternatively, one could also use a mean of the soundings within each cell. However, the soundings have already been spatially constrained through the inversion and so this choice will not have a large impact on the outcome. An example of the gridded resistivity data is seen in Figure 8-2.

From the detailed surface geology (1:25.000), a map of the surface lithology is available (Jakobsen & Tougaard, 2020). This map consists of polygons separating the top surface of Denmark into lithologies. The surface geology map is transferred to grid cells using the lithology of the polygon corresponding to the grid cell coordinates in GIS. The lithologies are then grouped according to the lithology grouping decided in the geology TI process as described in Table 6.1. The discretized and grouped surface geology map is then transferred to the top cells in the simulation cell. Because the borders between polygons come with some uncertainty, we remove all surface geology map nodes that do not share a common lithology group with its eight surrounding neighbours, thus creating a buffer zone along the borders of the polygons.

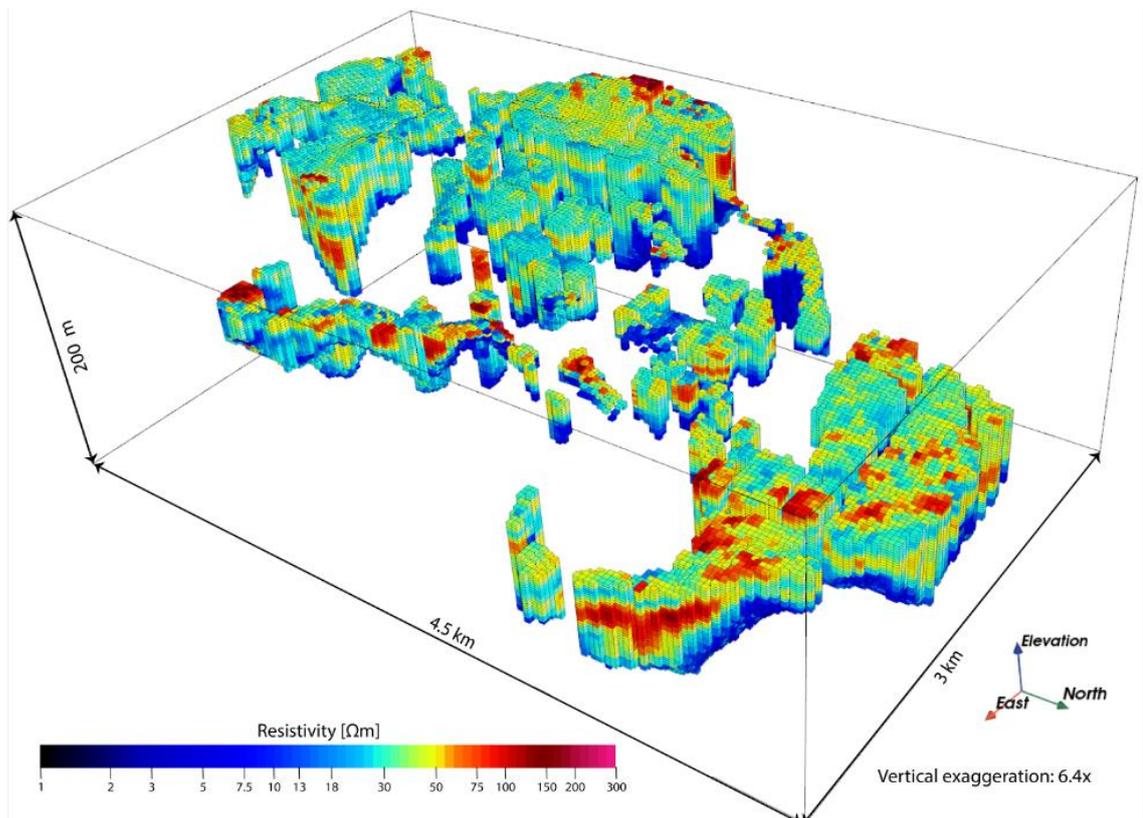


Figure 8-2: Gridded resistivity data in LOOP3 (Madsen et al., 2021a).

Finally, the geology and wells containing interpreted information on redox conditions (“redox wells”) in the area are placed in the simulation grid. The geology wells can be retrieved from the Jupiter database with a lithological description for all intervals of the wells. As for the surface geology map, these lithologies can be grouped according to the convention. The wells are then discretized into the vertical grid spacing. The most abundant lithology group within each grid cell is chosen to represent the entire cell. If, for instance, a cell is made up of 80% meltwater clay and 20% meltwater sand, the cell is represented entirely by meltwater clay. Lastly, all geology wells are placed in the simulation grid at the grid cell nearest to the well coordinates. If the lithology group of the top cell of a well is conflicting with the surface geology map, the surface geology map is chosen over the well.

The redox wells are interpreted and split into the three distinct redox categories – 1) oxic, 2) N-reducing and 3) reduced conditions. This interpretation is based on sediment colour descriptions from the Jupiter database and sometimes also on water chemistry depending on the availability of such information (see also Chapter 7). The interpretation is discretized into the vertical spacing of cells, such that the wells can be placed directly into the simulation grid.

8.2 Prior simulations and iterative sampling setup process

In DS the conditional probabilities are not computed directly but are instead sampled by scanning the TIs for a matching event each time the algorithm visits a new node in the simulation grid. A set of algorithm parameters needs to be set to control how the scanning is

performed. The tuning of these algorithm parameters will ultimately affect the final simulation output. Consequently, the prior information in the geostatistical system is thus made up of the TIs and how this is translated into conditional probabilities (i.e. the choice of MPS sampling algorithm and its parameterization). Thus, the structural input from the geologists and geochemists is not limited to creating the TIs and delineating the area in GEs. Instead, in the proposed workflow we suggest an iterative process like that proposed in Høyer et al. (2017) where realisations from the prior model are generated to visually see whether the actual structures presented match the expectation of the system. If not, either TIs or sampling algorithm parameters can be changed until a satisfactory result is achieved. In this iterative process one should also include considerations on the computational feasibility of the chosen parameterization.

Given the small size of the TIs images compared with the simulation domain two very important parameters are needed to be set relating to the computational speed. Firstly, the fraction of the TI that needs to be scanned until a reasonable match is found needs to be set. Due to the small TI sizes, we suggest scanning the entire TI for a match, which is statistically most reasonable to create the full conditional probabilities and does not take unnecessary amounts of additional computation time. Secondly, since MPS is based on patterns between several points, the number of already simulated points to include in the search event during each iteration needs to be set. For a small number of points, the variability in the system is large and computes fast, however this happens at the expense of losing larger structures and trends displayed in the TIs. Here the strategy of prior visualization is important to justify the trade-off between the representation of spatial patterns and the computational speed. See Madsen et al. (2021a) for a more in-depth analysis of this procedure.

The prior configuration that satisfied the above criteria in LOOP3 are visualized through two prior realisations in Figure 8-3.

8.3 Establishing resistivity-lithology relationship

Resistivity-lithology relationships need to be established such that resistivities are relatable to geology. Because a specific lithology grouping is chosen, a relationship specific for these groups needs to be established. Here, the geology TIs are used to infer the resistivity-lithology relationship. As outlined, the geology TIs are made within the simulation domain based on the tTEM models and other available data sources. Hence an implicit resistivity-lithology relationship is already in place and is used in the geological modelling. This relationship can be inferred by building histograms of the resistivities for each lithology group. For each of the lithology groups in the TIs, the corresponding resistivity values in the simulation grid are used to build these histograms. Specifically, if a resistivity value exists for a given grid cell containing a lithology value in the TI, this resistivity value is then associated with the given lithology group in the TI. If only a few counts of resistivities exist for a given resistivity value for all lithology groups, a background resistivity-lithology relationship based on the regional characteristics of the lithology groups is used. The reader is referred to Madsen et al. (2021a) for more details on the inference procedure.

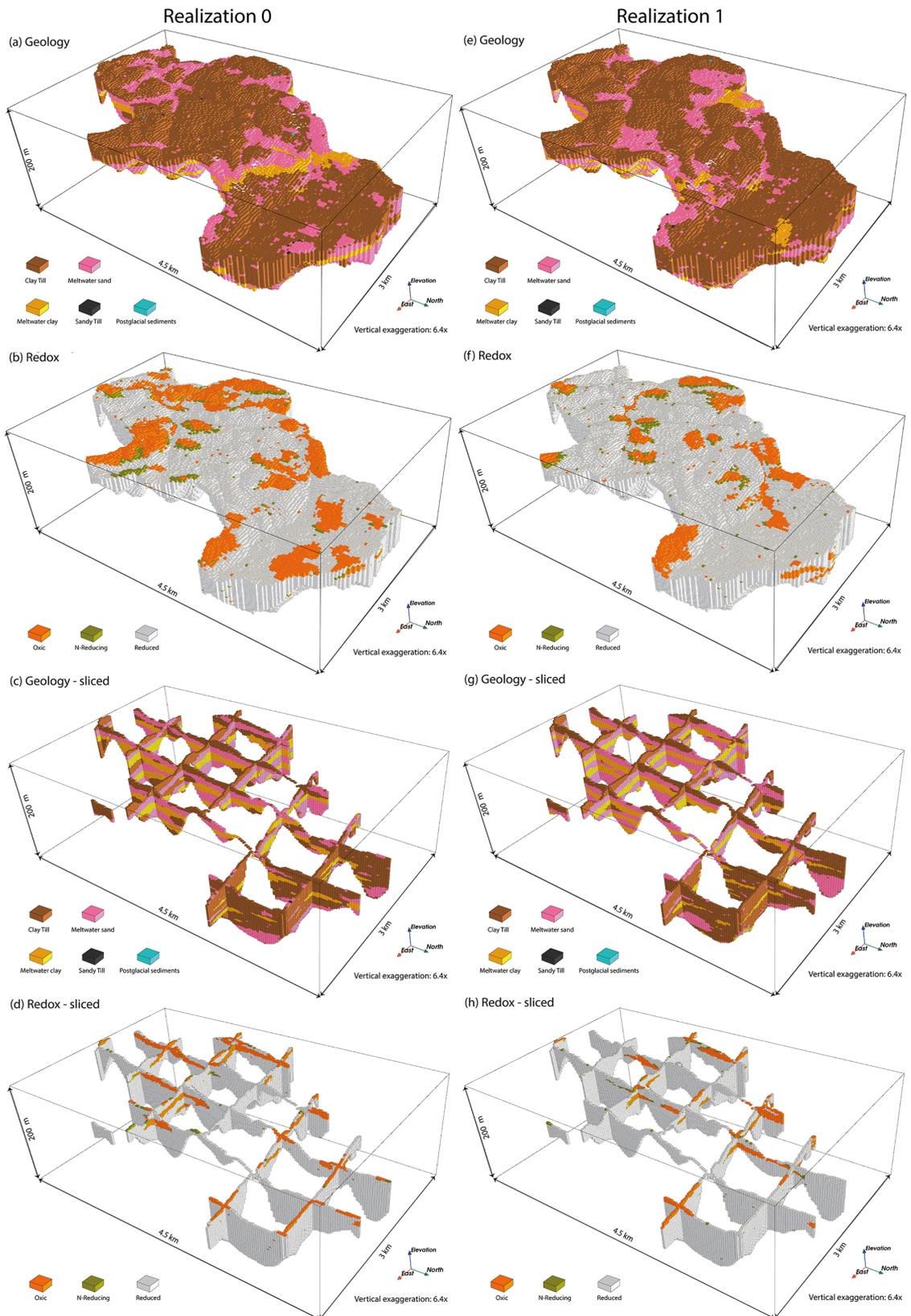


Figure 8-3: Two realisations from the prior model. (a, b) One realisation of jointly simulated geology and redox. (c, d) The same realisation represented as a fence diagram with slices in the x and y direction. (e–h) Same figure configuration as in (a–d) but for a different realisation. (Madsen et al., 2021a).

8.4 Conditional data

The discretized well and surface geology information is placed directly in the simulation grid as outlined previously. This means that these values cannot change throughout the simulation between individual realisations. Data are therefore known as hard data. These nodes typically are the nodes to form the first conditional events to which a matching event in the TI is to be found during simulation.

The established resistivity-lithology relationship allows us to map the prior probabilities of each lithological group based on the tTEM in the area. These probabilities are known as soft data probabilities and are used as conditional data in the simulations. Because the resistivity-lithology relationship is based on the TIs, the prior information will be consistent with these soft data probabilities. When simulating, the values tend to match the values in the TI and the general mismatch between the training image patterns (since it is based on actual geology) and the tTEM data is minimized. Conversely, this puts a lot of confidence in the work carried out in the TIs.

Soft data probabilities are also derived from the surface geology map in the buffer zone at the top cell where there is no hard data. These probabilities are based on the value from the surface geology map. The lithology group from the surface geology map is given highest probability and the remaining probability (summing to one) is spread equally across the remaining other lithologies. As an example: The grid node value of the surface geology map indicates meltwater clay, however the surrounding neighbours are not all meltwater clay. Therefore, the grid node is not treated as hard data, but we want to convey that it most likely is meltwater clay in this grid cell. We assign a probability of e.g. 0,8 to meltwater clay and the remaining 0,2 is distributed amongst the other lithology groups. Hence, the most likely outcome from the soft data probabilities is meltwater clay in this cell, but also allows different lithologies to appear in the simulations.

The surface geology map is also used to make soft data probabilities for redox in the top cells of the simulation. Here, the conversion probabilities for the three redox categories are based on the available well information in and around the simulation grid. The probabilities oxic, N-reducing, and reduced for sand (i.e., meltwater sand/gravel and sandy till) were 0.6, 0.2, and 0.2, respectively, and those for clay were 0.8, 0.1, and 0.1. Postglacial sediments, which are organic matter rich, are exclusively in reduced condition: 0.05 (oxic), 0.05 (N-reducing), and 0.9 (reduced); (Madsen et al., 2021a). The conversion probabilities for LOOP3 are described in section 7.3.

8.5 Posterior simulations

The prior information of the system (geology and redox TIs as well as the algorithm parameterization) is combined with the conditional data for each GE. Using joint geostatistical MPS simulation, realisations of the subsurface geology and redox are generated simultaneously. These combined realisations are independently simulated and hence represent a sample of the posterior model. In the current setup, sample sizes of 100 individual realisations seems to be a reasonable estimate of the posterior distribution of the spatial variability of geology

and redox, while remaining computationally feasible on a personal laptop. The posterior models of the individual GEs are also simulated independently of each other. Thus, the set of posterior models for each GE can be combined into a posterior model for the entire area to create the final posterior model. An example of posterior realisations from LOOP3 can be seen in Figure 8-4.

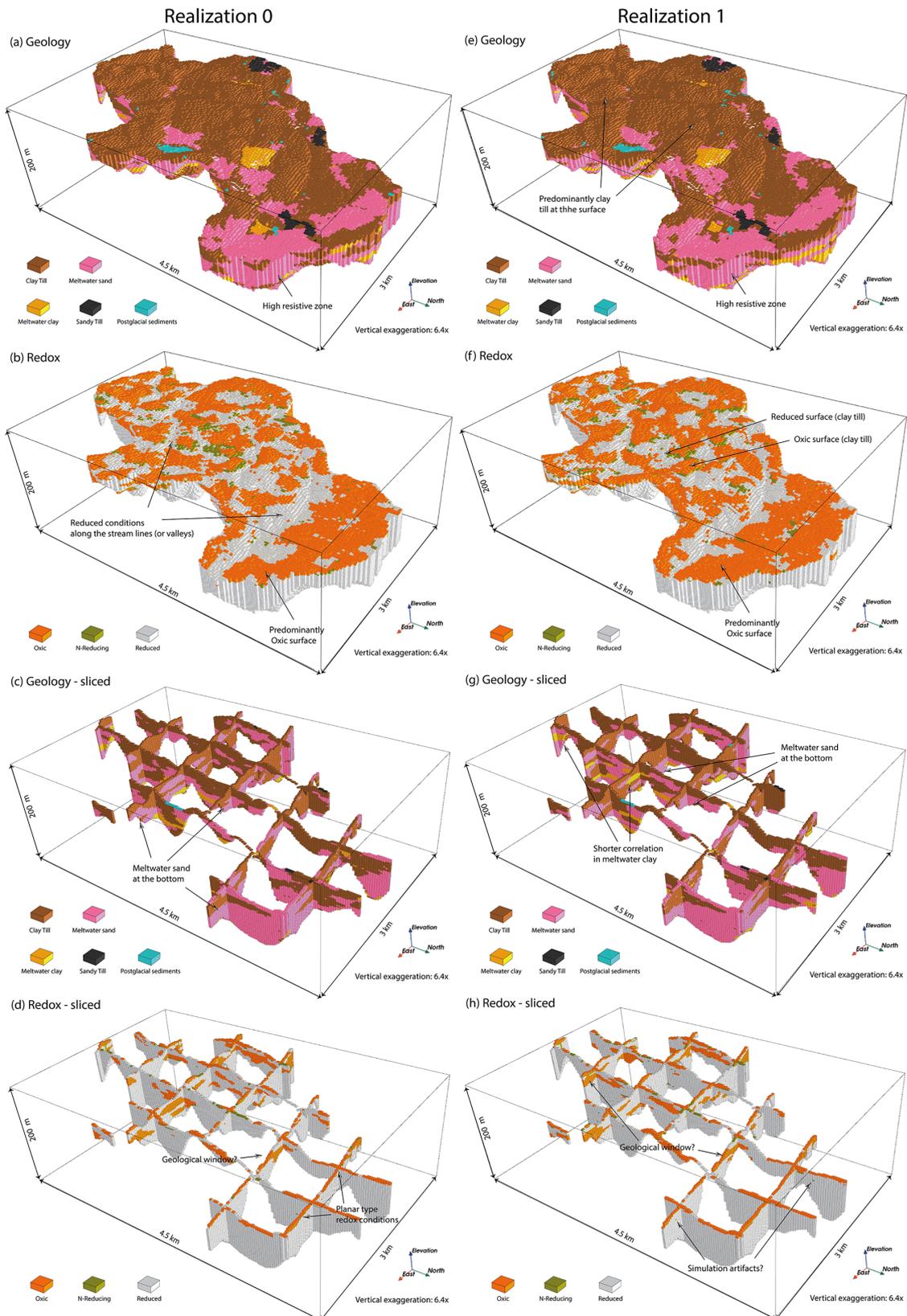


Figure 8-4: Two realisations from the posterior model. (a, b) One realisation of jointly simulated geology and redox. (c, d) The same realisation represented as a fence diagram with slices in the x and y direction. (e-h) Same figure configuration as in (a-d) but for a different realisation. (Madsen et al., 2021a).

9. Modelling output

The final output from the described workflow will be modelling results and documentation:

- 1) **A digital 3D geological model:** A GeoScene3D project including all data, interpretation points, gridded surfaces of the boundaries of each geological element, and geochemistry data.
- 2) **A geochemical model:** 1D interpretation of geochemical data in new wells, combined 2D interpretation along profiles including a conceptual model of redox architectures, TI's of redox condition and denitrification rates related to lithologies.
- 3) **Stochastic modelling realisations:** All model realisations of each geological element combined to overall realisation outputs for distribution of lithologies and redox architecture.
- 4) **Standardised documentation:** A final report including descriptions of data, decisions, interpretations, a qualitative assessment of the uncertainties of the GE boundaries and a quantitative uncertainty assessment on the MPS modelling of the GEs – both geology and geochemistry.

10. Conclusions and perspectives

10.1 Conclusions

This report describes a Geological Elements modelling approach developed at Department of Groundwater and Quaternary Geology Mapping at GEUS for the MapField project. The approach introduces co-interpretation and integration of geostatistical simulation of geological and redox structures and is based on combining existing data with detailed geophysical mapping of the upper subsurface. The newly developed geophysical tTEM method is combined with a field campaign acquiring central point data of sediment and water samples for geochemical analysis as well as lithological descriptions. Redox conditions, and the potential denitrification rates are closely related to the geology and hydrogeology. Therefore, a joint approach handling both modelling of the geological architecture and modelling of redox architectures have been developed. The output is intended for use in the subsequent hydrological modelling with N transport and turnover using the MapField concept (<https://eng.map-field.dk/>).

The Geological Elements approach has been developed as a versatile tool that ensures that geophysical and geochemical data are co-interpreted with geological data and knowledge. The advantage of this approach is that gained geological knowledge from both inside and outside the target area constitutes a foundation for the interpretations of redox conditions and groundwater flow. The concept tool is basically a workflow leading through a series of tasks, which can be individually adjusted based on the physical and geochemical conditions of the specific area and the needed output from the modelling. The concept combines manual and semiautomatic procedures where an understanding of the hydrogeological and geochemical setting is paramount.

One of the main strengths of the Geological Elements approach is its flexibility enabling adjustments of the individual parts. No two areas are alike and therefore ongoing assessments of results can be used to adjust the level of work in each task. Generally, by using the Geological Elements approach, the geological modelling part is simplified and thereby the time used for constructing a 3D geological model is minimized. Geological complexity at metre-scale is revealed in the geophysical data, and consequently, modelling methods and approaches should be designed to handle this high level of spatial detail. In order to address this, cognitive 3D geological modelling is combined with statistical simulations and in addition to this geological and redox structures are co-interpreted.

The Geological Elements approach has been applied, modified, and evaluated in four LOOP pilot areas with different geological settings leading to the following scientific highlights:

- The ***tTEM mapping contributes with new details of the subsurface***, primarily down to 30-50 m's depth, which significantly improves the geological understanding of the upper subsurface, but also links to a better understanding of the deeper geological succession in combination with existing knowledge.

- The geological architecture has been interpreted and delineated in each pilot area, highlighting that even ***a limited interpretation effort heightens the understanding of the tTEM results*** and leads to an improved interpretation of the geological event chronology.
- **Iterative integration of knowledge** of geological structures and redox architectures strengthens the interpretation of the subsurface conditions from point to catchment level.
- The ***delineation of geological elements*** is done by point interpretation and interpolation of 2D grid surfaces in the software GeoScene3D. The ***geological Training Images (TI)*** are modelled as 3D voxel grids with a specific size (volume) and lithology group, and subsequently implemented in the geostatistical workflow.
- **Building a redox TI based on the geological TI** is efficient and scientifically sound due to the co-interpretation of geology, hydrogeology and redox conditions.
- The representativeness, density, and quality of the geochemical data is key to lowering the uncertainty of the geochemical modelling. Hence ***prior knowledge of the geological and hydrogeological structures is paramount for designing cost-efficient field campaigns for geochemical investigations.***

10.2 Perspectives

The described Geological Elements approach of the MapField concept can be used in groundwater modelling with N transport and turnover for the preparation of N retention maps at field scale. The Geological Elements approach constitutes a way of integrating both geological and redox information into geostatistical modelling which is a further development of Vilhelmsen et al. (2019), where lithology is modelled using MPS simulations using training images based on accumulated clay thickness combined with clustering.

In the Geological Elements approach, it has been very important to maintain a high level of detail in all steps of the workflow. However, the need for detail in 3D geological/hydrogeological models is not a new thing, but until the development of the tTEM method, mapping of 3D geological complexity in the uppermost 50 meters and at meter-scale was difficult to obtain.

With the tTEM method, the possibilities for high-detail 3D models are now at hand, and with the Geological Elements approach of the MapField concept, the new type of 3D mapping and modelling has the potential to be used in many other project types which face a variety of subsurface challenges. Geo-energy projects dealing with the upper subsurface, mapping of onshore raw materials, and climate adaptation related projects, are all aimed at detailed understanding of the geology, the hydrology, and the geochemistry in order to obtain the best basis for decision-making.

Vulnerability assessments of groundwater resources

Mapping of aquifer vulnerability aimed at securing drinking water resources is obviously challenged by a general lack of detailed and dense datasets. The joint modelling approach is highly relevant as it can handle large datasets and because it embraces both geological and geochemical key parameters resulting in more detail and precision than previously achieved.

Mapping and modelling of contaminated sites/contaminated groundwater

Modelling pathways of contaminants from point sources and into the subsurface also require detailed 3D models. Assessments of point sources in the open land whether they be industrial sites or contaminated sites related to agricultural activities could benefit from the Geological Elements approach for mapping and modelling the natural protection in the uppermost part of the subsurface.

In many cases, however, contaminated sites are situated in or close to an urban area where mapping with tTEM will be impossible because the method can be affected by man-made installations. The primary dataset in these cases will be boreholes, but nevertheless, the MapField approach is attractive in these cases as well, as GEs and TIs (based primarily on boreholes in this case) will add both significant value and time reduction in contrast to a fully manual approach.

Multi-purpose 3D geological models

Local, regional, and national authorities deal with many types of challenges related to the subsurface, and in many areas existing low-resolution models can maybe give a geological overview, but not a thorough geological understanding of a given area. The Geologic Elements approach can be used for construction of geological models, which by the combination of cognitive and semiautomatic approaches can produce geological models that provide a general geological understanding, and at the same time is able to incorporate all existing data into a statistical model. A great advantage is, that this type of model can easily be updated when new data is available. 3D geological models constructed using the Geologic Elements approach will include a limited number of GEs but will by using statistics incorporate all available data. In this way, a preliminary spatial geological model can be produced. This type of model will provide an overview and an understanding of the geological architecture to be used for the planning of future mapping projects.

Climate-change related projects

Many climate-related projects concern falling or rising groundwater levels, and for instance when forced infiltration is the only solution, very detailed local models are needed. Detailed hydrogeological models will be able to point to suited infiltration areas and subsequent hydrogeological modelling will provide calculations of water volumes and probable pathways of the infiltrated water.

Raw material mapping

The tTEM method is very good for mapping aggregates such as sand and gravel. The Geological Elements approach can potentially be used for both assessments of resources and for modelling hydrological and geochemical impacts on groundwater and surface waters from projected quarrying.

Geo-energy projects

The shallow subsurface is in many areas a potential resource of sustainable energy. To utilise this resource in energy related projects, such as establishing an Aquifer Thermal Energy Storage (ATES) system or Borehole Heat Exchangers (BHE) for heating or cooling, a thorough understanding of the geology, hydrogeology, and groundwater chemistry is essential in the feasibility and investigation phases. This is necessary in order to configure, model and

predict the performance of a planned geo-energy system related to the surface energy demands. The presented modelling concept will be highly relevant in especially ATEs projects where thermal and geochemical modelling is required and should be based on a detailed subsurface 3D model. The workflow should of course be adapted for the specific site as local conditions, for instance, could require a different approach in the data collection phase.

Utilization and further end-user optimised improvement of the joint modelling concept will likely generate an expanding suite of detailed models. With the MapField project as a starting point, this will support the build-up of a database with TIs describing different local geological and geochemical settings. Potentially, the future TI modelling process will gradually be more effective as dedicated TI builders with a database of TI starting cubes (existing models) can ease the modelling task and decrease time consumption when designing TIs. Likewise, a better description of the local geological event chronology will create a positive spin-off on the interpretation of both geology and geochemistry at a regional scale.

Independent of the specific purpose of a subsurface/groundwater project, geological and geochemical knowledge is still important in order to relate and implement local mapping results in a regional context. An overall understanding of the geology and the geochemical parameters is hence considered a prerequisite for obtaining robust modelling results.

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