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Nitrate reduction in geologically heterogeneous catchments — A framework for assessing the scale of predictive capability of hydrological models

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HIGHLIGHTS

- We develop a new airborne geophysical measurements — Mini-SkyTEM.
- We identify geological structures with 2 m vertical and 30–50 m horizontal resolution.
- We describe geological uncertainty by TProGS conditioned by geophysical data.
- We assess subsurface nitrate reduction using distributed hydrological models.
- We assess the minimum scale of predictive capability of the hydrological model.

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ABSTRACT

In order to fulfil the requirements of the EU Water Framework Directive nitrate load from agricultural areas to surface water in Denmark needs to be reduced by about 40%. The regulations imposed until now have been uniform, i.e. the same restrictions for all areas independent of the subsurface conditions. Studies have shown that on a national basis about 2/3 of the nitrate leaching from the root zone is reduced naturally, through denitrification, in the subsurface before reaching the streams. Therefore, it is more cost-effective to identify robust areas, where nitrate leaching through the root zone is reduced in the saturated zone before reaching the streams, and vulnerable areas, where no subsurface reduction takes place, and then only impose regulations/restrictions on the vulnerable areas. Distributed hydrological models can make predictions at grid scale, i.e. at much smaller scale than the entire catchment. However, as distributed models often do not include local scale hydrogeological heterogeneities, they are typically not able to make accurate predictions at scales smaller than they are calibrated. We present a framework for assessing nitrate reduction in the subsurface and for assessing at which spatial scales modelling tools have predictive capabilities. A new instrument has been developed for airborne geophysical measurements, Mini-SkyTEM, dedicated to identifying geological structures and heterogeneities with horizontal and lateral resolutions of 30–50 m and 2 m, respectively, in the upper 30 m. The geological heterogeneity and uncertainty are further analysed by use of the geostatistical software TProGS by generating stochastic geological

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realisations that are soft conditioned against the geophysical data. Finally, the flow paths within the catchment are simulated by use of the MIKE SHE hydrological modelling system for each of the geological models generated by TProGS and the prediction uncertainty is characterised by the variance between the predictions of the different models.

1. Introduction

Excess nitrogen from agricultural fertilisers and manure constitutes a significant environmental problem in many regions of the world (Kronvang et al., 2009a). This is also pertinent for Denmark, where nitrate leaching from agricultural areas is one of the major water resources management problems. Nitrate load from agricultural land to lakes and coastal water in Denmark has during the past 25 years been reduced by about 50% by government regulations imposed on agricultural practice. The EU Water Framework Directive, WFD (European Union, 2000) will require an additional reduction of nitrate load by about 40%, which economically will be very costly for the agricultural sector. The regulations imposed until now have been uniform, i.e. the same restrictions for all areas independent on the subsurface conditions. Studies have shown that on a national basis about 2/3 of the nitrate leaching from the root zone is reduced naturally, through denitrification, in the subsurface before reaching the streams (Ernstsen et al., 2006; Hansen et al., 2009). This implies that if a uniform agricultural regulation reduces nitrate leaching by 100 kg N, the nitrate load to surface water will only be reduced by 33 kg N. Therefore it would be more cost-effective to identify robust areas, where nitrate leaching through the root zone is reduced in the saturated zone before reaching the streams, and vulnerable areas, where no subsurface reduction takes place, and then only impose regulations/restrictions on the vulnerable areas (Jacobsen, 2012; Ørum and Jacobsen, 2013; Natur- og Landbrugskommission, 2013).

Hydrological models have for many years been recognised as useful tools for catchment scale simulation of nitrate loads from agricultural areas (Styczen and Storm, 1993a, 1993b; Whitehead et al., 1998; Refsgaard et al., 1999; Arheimer and Brandt, 2000; Conan et al., 2003). The EUROHARP study (Schoumans et al., 2009) showed that eight different models, calibrated against field data, were able to simulate annual nitrate loads satisfactorily, and they performed almost equally well for a wide range of catchments. However, Kronvang et al. (2009b) showed that although the eight models had similar performance for simulation of annual net catchment loads, there were considerable variations among the models with respect to the internal fluxes and processes such as point sources, diffuse sources, denitrification and reduction in subsurface and surface waters, i.e. that the eight models generally produced the right answers, but not necessarily for the right reasons.

In order to provide support for management decisions on identifying areas that are robust and vulnerable, respectively, with regard to nitrate load in a Danish context, models have to fulfil two additional requirements compared to state-of-the-art in catchment scale nitrate modelling: (i) the models must have predictive capability at small spatial scales, preferably 1 km^2 or below; and (ii) the models must be able to simulate nitrate reduction in groundwater systems, as most of the nitrate reduction occurs here due to the groundwater dominated hydrological regime with shallow redox interface, small river systems and relatively few and small lakes.

To meet these requirements distributed hydrological models, which consider 3D groundwater flow and reactive transport, are required. Distributed hydrological models can make predictions at grid scale, i.e. at much smaller scale than the full catchment. Hence these models have a potential for being able to differentiate between robust and vulnerable areas. However, in all previous studies it has not been documented that distributed models have predictive capability at scales much smaller than the (catchment) scale at which they are calibrated (Hansen et al., 2008, 2009, 2013). The most important constraint in this respect is probably that distributed models often do not include local scale hydrogeological heterogeneities that are known to control reactive transport.

The information on geological heterogeneity at the appropriate scale can be greatly improved by applying geophysical methods such as SkyTEM (Sørensen and Auken, 2004; Viezzoli et al., 2009; Auken et al., 2009), a transient airborne electromagnetic (AEM) method. The development in transient AEM has over the last decade focused on systems with very high transmitter moment in order to resolve deep-lying mining targets or groundwater resources (Allard, 2007). These techniques, however, have a limited resolution of the geological structures and lithology, which in our case is particularly important for the surface near units, because this is where most of the water flow and associated nitrate reduction occurs. Furthermore, irrespective of the amount of available field data and information, lack of data will always remain a limiting factor for describing geological and geochemical heterogeneity deterministically. In this respect geostatistical approaches with stochastically generated geological realisations (Carle et al., 1998; Strebelle, 2002) may be useful tools, both for combining geological information from boreholes and geophysics and for assessing geological model uncertainties.

This raises the question about identifying the scale at which the local patterns are integrated sufficiently to produce similarity in response. At small scales, i.e. scales smaller than the length scale of structures possible to describe deterministically, differences in the actual pattern of the structures for different areas at this scale will produce different responses, even if the underlying distributions are identical. As the scale increases, more and more of the variability in the distributions is sampled within each area, and at some length scale all areas will yield almost identical responses. This large scale is defined by Wood et al. (1988) and Beven (1995) as the Representative Elementary Area (REA). For cases, where we do not know the exact spatial configuration of the properties, but only their statistical characteristics, the REA can be considered as the minimum scale at which a model potentially has predictive capabilities.

The objective of the present paper is to describe a new framework for assessing nitrate reduction in heterogeneous geological environments and for assessing at which spatial scales distributed hydrological models can have predictive capabilities.

2. General approach

The new framework has been developed in the NiCA project (www.nitrat.dk). An essential element is the incorporation of uncertainties on geology and its implication for uncertainty on hydrological model predictions using the definitions of uncertainty from Refsgaard et al. (2007). The framework, illustrated in Fig. 1, comprises the following key elements:

1. *Airborne geophysical mapping with high spatial resolution*. To provide best possible information on geological heterogeneity over large areas airborne geophysical mapping is carried out. The main output is geophysical soundings with a spatial resolution of 1.5–3 m vertically and 30–50 m horizontally in the uppermost 30 m of the subsurface.
2. *Geological modelling with focus on geological uncertainty*. Geological modelling is carried out in two steps. First, a geological model, which delineates dominant large scale geological units, is developed.

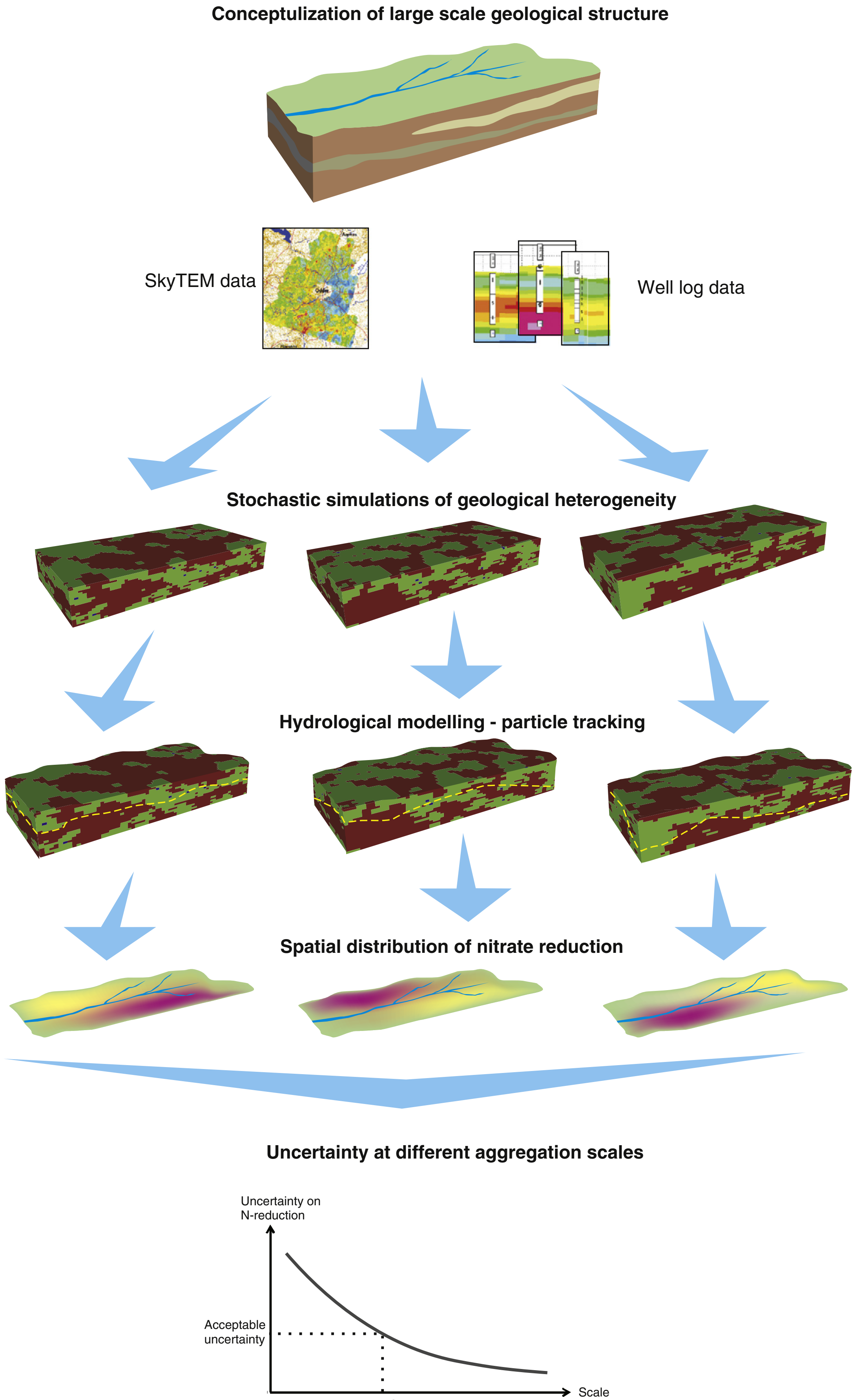

Fig. 1. Key elements in approach for assessing the scale of potential model predictability (RES).

Next, the small scale heterogeneity within the large scale geological units is described by use of geostatistical tools using information from both borehole data and geophysical data. The output from this step is a number of plausible geological realisations.

3. *Characterisation of redox interface in the saturated zone*. The basic hypothesis for the nitrate reduction is that no reduction takes place in the oxic zone between the bottom of the root zone and the redox interface, while all nitrate passing below this interface is immediately reduced. This makes nitrate reduction in the subsurface only dependent on the flow paths and the location of the redox interface. Recognising that it is not feasible to obtain sufficient field data to describe the redox interface deterministically at local scale, it is described statistically on the basis of field data and modelling studies.
4. *Hydrological modelling with particle tracking*. Coupled surface water/ groundwater models are established for each of the geological realisations/models (Step 2) and autocalibrated inversely against available groundwater head and river discharge data. Flow pathlines are simulated for each of the geological models to assess the fraction of the pathlines originating from a given surface grid that are passing the redox interface.
5. *Assessing the scale of potential predictive capability — the Representative Elementary Scale (RES)*. The uncertainty on the predictions of nitrate reduction from a surface grid is assessed on the basis of the differences in predictions among the models originating from different geological realisations (Step 2). By aggregating results from an increasing number of model grids a curve showing the relationship between length scale and uncertainty can be derived. The smallest scale, where the uncertainty is below a given acceptable uncertainty level, is denoted the Representative Elementary Scale (RES).
6. *Use of the concept in water resources management*. The perspectives of applying a differentiated regulation of agricultural production, instead of the traditional uniform regulation, will be assessed economically through a process of active stakeholder involvement.

3. Study sites

The concept is tested in two areas:

- The 4.7 km^2 Lillebæk catchment located on the island of Funen, Denmark. Lillebæk catchment has been monitored since 1989 as part of the Danish Agricultural Watershed Monitoring Programme (LOOP-programme), which was established in order to evaluate the agricultural pollution of the aquatic environment (Rasmussen, 1996). The monitoring has focussed on the fate of nutrients and the concentrations in soil water, upper groundwater, tile drains and streams.
- The 101 km^2 Norsminde catchment south of Aarhus in Jutland, Denmark. This catchment has average data coverage with respect to long time series, but several agriculturally related research projects have been initiated in the catchment during the past few years. A particular advantage of the Norsminde area is that a very constructive working relationship has been established with local farmers through these projects.

The land use in both catchments is dominated by intensive agriculture, and both catchments are situated in young glacial landscapes dominated by glacial clayey till soils. The flow pathlines are illustrated in the conceptual sketch in Fig. 2. The flow pathlines are influenced by tile drains, located at around 1 m depth, and nitrate reduction is governed by the spatial configuration of the flow pathlines and the location of the redox interface. Of critical importance for the fate of nitrate is whether or not the pathlines are intersecting the redoxfront.

4. Methodologies

4.1. Geophysical data

In transient Airborne ElectroMagnetic (AEM) methods a primary magnetic field generated by a transmitter loop carried by an airplane or by a helicopter is emitted (Fig. 3, left). After abrupt turn-off of the current in the loop, inductive eddy currents occur in the ground, which generates a secondary magnetic field. The decay of this field depends on the resistivity of the geological layers. Compared to other transient AEM systems, the SkyTEM system (Sørensen and Auken, 2004) has the particular feature that measures the responses from two different moments during the same survey. The Super Low Moment (SLM) is suited for mapping the near surface part, while the High Moment (HM) is aimed for resolving deep structures (see typical sounding curve in Fig. 3, right).

A new version of the SkyTEM system, referred to as Mini-SkyTEM or SkyTEM101 has a smaller transmitter loop (130 m^2) compared to the other SkyTEM systems (up to 500 m^2). The carrier frame is constructed

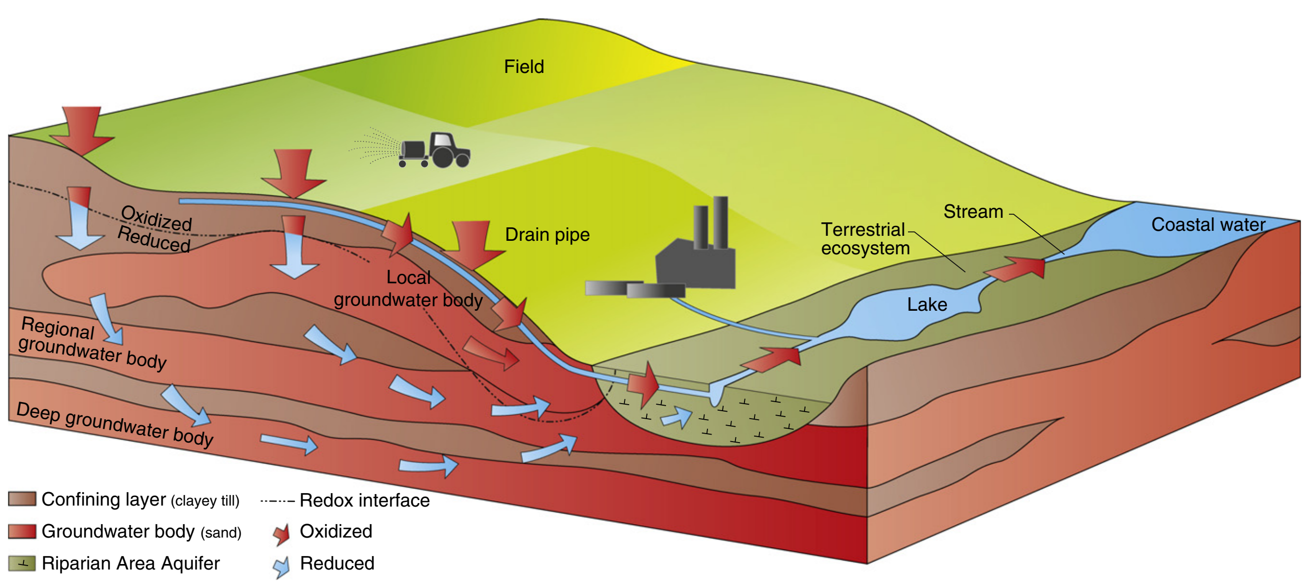

Fig. 2. Flow paths, redox interface and nitrate reduction in Danish glacial till area. Modified from Hinsby et al. (2008).

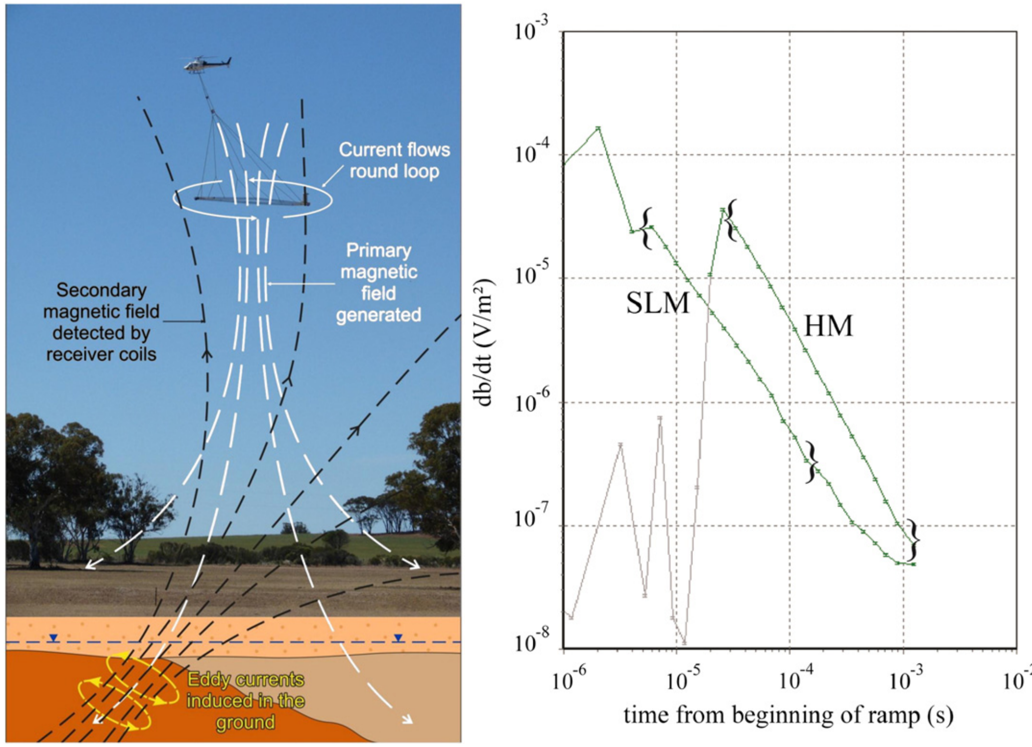

Fig. 3. Transient Airborne ElectroMagnetic concept. Left: a primary field is generated with the transmitter frame hold by the helicopter. When the primary current in the loop is turned off, the ground responds with a secondary magnetic field which depends on the resistivity distribution. Right: a typical sounding curve measured by the new Mini-SkyTEM system. Two moments with different intensities are measured: the Super Low Moment (SLM) for the early times and near surface information and the High Moment (HM) for late gates and deep inverstigation. The brackets indicates the times used for the geophysical interpretation.

with an aerodynamic profile giving a small drag in the air, thus making the system easy to fly in a nominal altitude of 30 m. The improved near-surface resolution is made possible by the small carrier frame together with a tailored transmitter system allowing for a very short turn-off of 3 μs using a current of 7.5 A. The large penetration depth of down to 100–130 m depending on the geology (Christiansen and Auken, 2012) is obtained by the high moment of the system transmitting 55 Amp. With a sounding sampling of 0.6 s and a flight speed of 100 km/h the best lateral resolution from the raw data is 15 m. However, gentle stacking of the late time data is necessary, and after processing the lateral resolution is in the range 30–50 m for the top 30 m.

4.2. Geological heterogeneity and uncertainty

The geology in the two areas is divided into large scale structural elements. In the Norsminde area they include an upper Quaternary glacial sequence, a Miocene sand/clay sequence, buried tunnel valleys and a glaciotectonic complex. The delineation of structural elements has been carried out by an experienced geologist by use of all available borehole and geophysical data. Also background knowledge on the geological processes that governed the deposition and erosion of sediments in this area during the Neogene and Quaternary periods is utilized.

The structural geological elements are quite heterogeneous internally. For instance, it is evident both from borehole and geophysics data that the upper glacial sequence contains clay till and lenses of melt water sand in highly irregular patterns. For each of the structural elements several plausible geological realisations of the internal small scale geological heterogeneities are generated by use of TProGS (Carle et al., 1998). For this purpose each borehole is characterised into five groups ranging from very high quality to unreliable. The high quality borehole data are used for hard conditioning, while the groups with less reliable data are used for soft conditioning. Furthermore, the borehole data from the very high quality group(s) are compared with geophysical sounding to establish a statistical relationship between resistivity (output variable from SkyTEM) and probability of sand or clay (Gunnink and Siemon, 2009; Gunnink et al., 2012). This relationship is then used for soft conditioning of the geophysical data in TProGS.

4.3. Redox interface

Based on previous studies it is assumed that no reduction takes place in the oxic zone between the bottom of the root zone and the redox interface and that nitrate reduction below the interface occurs at a much faster rate than the oxygen movement (Postma et al., 1991; Ernstsen, 1996; Ernstsen et al., 1998). Furthermore, it is assumed that the progression rate of the redox interface is so slow that the depth to redox interface can be assumed constant within a planning horizon of decades (Postma et al., 1991). The location of (depth to) the redox interface is critical for calculating the nitrate reduction. The existing national 1 km^2 map of redox interface depths (Ernstsen et al., 2006) is based on very sparse data (in average 2–3 data points per km^2). Given that this depth can be highly variable within few metres (Hansen et al., 2008) there are major uncertainties associated with assessment of the location of the redox interface. We are not aware of any geophysical technique or other feasible measurement techniques that can provide information on redox interface. As drilling of boreholes to describe the local scale variations is economically unrealistic in a practical water management context, we need to test other methods to derive information on the depth to redox interface from other existing data.

We hypothesize that the depth to the redox interface can be explained by the oxidation of reduced geological deposits due to transport of oxygen from the land surface since the last glaciation age. We will test this hypothesis by detailed hydrological modelling on a field site within the Lillebæk catchment, where we have detailed data on sediments from 31 boreholes. For this purpose we have chosen the HydroGeoSphere code (Therrien et al., 2008) which can handle 3D variably saturated flow patterns as well as flows in macropores and fractures that may be important for describing small scale heterogeneities in the depth to the redox interface.

Based on this hypothesis we use groundwater recharge data obtained by the catchment model and information on redox capacity of the different geological sediments to calculate a map with spatially variable depths to the redox interface. We then adjust this map using a calibration coefficient to the entire map, so that the total reduction for the entire catchment matches the difference between the nitrate leaching from the root zone and the nitrate flux measured at the river gauging station. The redox interface map is then assumed constant over time.

4.4. Hydrological modelling

The hydrological models for the two catchments are based on the distributed hydrological modelling system MIKE SHE (Abbott et al., 1986; Refsgaard et al., 2010a) which is set up on a 50 m grid for the Lillebæk catchment (Hansen et al., 2013) and on a 100 m grid for the Norsminde catchment. For the Norsminde catchment multiple hydrological models are constructed based on different geologies generated by TProGS. Each of these models are autocalibrated against groundwater head and discharge data using the inversion code PEST (Doherty, 2010). The modelling of flow paths is carried out by use of MIKE SHE's particle tracking module (DHI, 2011), where the number of particles released in a particular root zone cell is proportional to the time varying nitrate leaching in the root zone. On this basis the fraction of particles intersecting the redox interface becomes equal to the nitrate reduction fraction for this particular root zone cell.

To study the importance of tile drains for the split of flow into a horizontal component (tile drains without nitrate reduction) and a vertical component (recharge to aquifer system with possibility for nitrate reduction) modelling studies are carried out by use of the HydroGeoSphere code (Therrien et al., 2008) that can handle drains as line elements.

The nitrate leaching from the root zone is evaluated by an N-balance method, where the annual N leaching is based on existing agricultural management data reported from farmers to the authorities and the annual values subsequently converted to daily concentrations by use of water balances from MIKE SHE.

4.5. Scale of predictive capability — Representative Elementary Scale (RES)

The predictive capability of a model is here understood as the model's ability to predict state variables under conditions different from those applied during a calibration phase, e.g. changes in agricultural management. In rainfall-runoff modelling Wood et al. (1988) introduced the term representative elementary area (REA), denoting the minimum area at which only the statistical properties and not the actual distribution of parameters and input variables is important for the model results. Ignoring the actual spatial locations implies that the model only has predictive capability at a scale equal to or larger than the REA. We will use a generalised form of the term where area is replaced by scale, implying that the concept can be used for any scale in either space or time. The representative elementary scale (RES) is then the minimum scale at which a given model, at best, has predictive capability. In our case we hypothesise that the dominating source of uncertainty is the geology. We assume that the large scale geological structural elements can be determined deterministically, and that the uncertainty of the small scale geological properties can be described geostatistically by use of TProGS. The uncertainty on nitrate reduction originating from uncertainty on the small scale geology is then characterised as the standard deviation between predictions from multiple models generated by TProGS. As small scale uncertainties tend to balance out when aggregated to larger scales we expect to obtain a relationship between aggregation scale and uncertainty as shown by the curve at the bottom of Fig. 1.

4.6. Water management measures

The new developed tools will be applied in the Norsminde Fjord catchment in order to assess their usefulness in future water management planning. The catchment will be divided into robust and vulnerable areas and the uncertainty of this delineation will be assessed. The farmers in the area will be involved in evaluating the practical feasibility of a large range of possible measures to reduce the nitrate leaching. The economic analyses for the area will consist of three different scenarios:

- *Uniform regulations*. The costs of reaching a given reduction goal based on a general approach with no detailed knowledge of nitrogen losses at different locations will be calculated. The analysis will be based on the Ministry of Environment "blue nitrate map" that in practice implies that the subsurface reduction is assumed uniform over the entire catchment. Selected general measures proposed for the implementation of The Water Framework Directive will be applied (Jensen et al., 2009; Jacobsen, 2012).
- *Site specific regulations*. The costs of reaching a given reduction goal will be calculated based on estimated differentiated subsurface reduction capacities in the catchment. The measures will be the same as with uniform regulation (Ørum and Jacobsen, 2013).
- *Site specific, farmer based management*. This will be a new strategy, where local farmers are empowered to identify site specific measures that serve the dual purposes of optimising the farmers' total economic gains and the environmental goals within a catchment. The costs of reaching a given reduction goal will be calculated based on estimated differentiated subsurface reduction capacities and an action plan developed in close interaction with the individual farmers considering the most cost effective measures, the location of vulnerable/robust areas and Good Agricultural Practice. A range of measures with documented effects will be used.

The purpose is to compare the three scenarios in terms of costs, measures and location. Are there side-effects which allow for more benefits when the site specific issues are included in the planning? To what extent will farmer active participation give an effect which increases the cost effectiveness compared to the legislative approach? Together with the new knowledge about vulnerable and robust areas it will be possible to demonstrate the cost effectiveness of management planning on a detailed scale rather than on a more general catchment scale. The economic benefits of using more precise, local scale regulations compared to general approaches will be analysed as well as the advantage of including local farmers in the decision process.

5. Preliminary results

In the following sections some of the methodologies are illustrated by preliminary results from the Norsminde catchment.

5.1. Geophysical mapping

After data processing including removals of data points disturbed by man-made installations, e.g. buried pipes along roads or power lines, the data are inverted using a spatially constrained inversion scheme (Viezzoli et al., 2008; Auken et al., 2012; Kirkegaard and Auken, 2013) which provides a quasi-3D distribution of the ground resistivity. With almost 2000 line km and more than 100,000 sounding positions over the Norsminde catchment, the computation for 29 layers takes about one week on 40 processors. The line spacing between the flight lines is maximum 100 m, and almost all the western half of the survey area has been covered with 50 m line spacing, providing a data set in a dense regular grid.

Fig. 4 shows the mean resistivity map at the depth interval 15–20 m. The resistivity values in the Norsminde area range between 1–2 Ωm and 100–200 Ωm. The smallest values correspond to Paleogen clay and the largest values to sandy layers with almost no clay. Fig. 5a

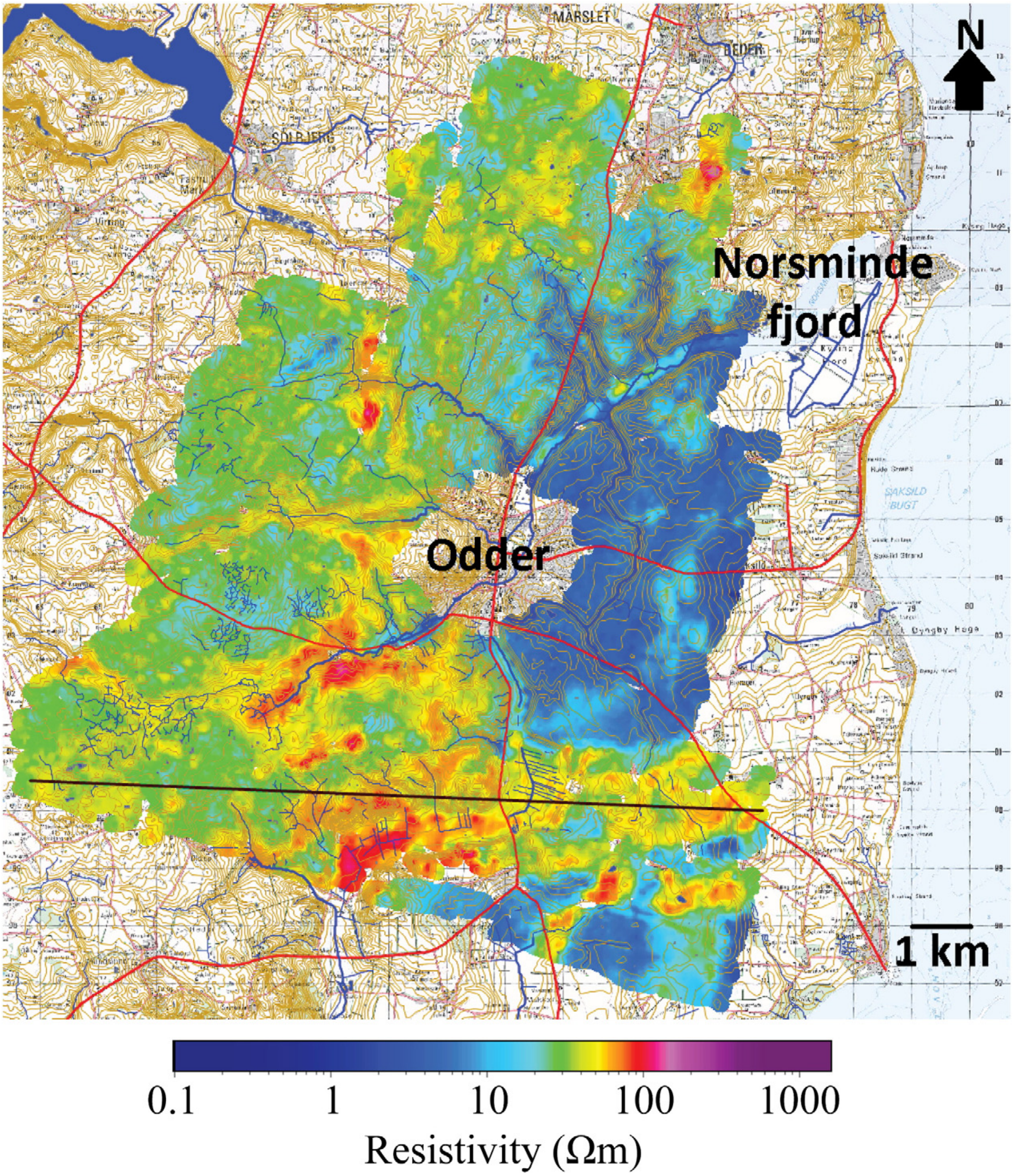

Fig. 4. SkyTEM results from the Norsminde catchment: Mean resistivity map of the depth interval 15–20 m. Results are obtained after a spatially constrained inversion with 29 layers from 1.5 m to 150 m depth. The map is obtained after kriging with a search radius of 150 m. Light brown lines correspond to topographical isolines, blue ones to streams, and red ones to main roads.

illustrates a section through the area with borehole log data inserted (only boreholes at a distance less than 50 m from SkyTEM flight lines are considered). Borehole data zooms of the western and eastern parts of the profile are given in Fig. 5b and c, respectively. This comparison shows very good correlation between the resistivity and the geology in the boreholes. A comparison study over the entire survey area with more than 35 good-quality boreholes closer than 50 m from the flight lines has shown very good correlation in 60% of the cases and acceptable matches for 30% of them. So only 10% of the boreholes show disagreements which could be explained by e.g. strong 3D lateral variations, quality of borehole data, location errors.

In the present sedimentary context all layers, mixtures of clays and sands, can be assumed to be saturated with fresh water.

5.2. Stochastic geological modelling

The overall geology in the Norsminde catchment has been delineated into seven large scale structural elements, some of which cover glacial deposits, while others represent deeper, underlying deposits. Most of the elements only cover part of the catchment area. TProGS is applied to generate geological realisations of the upper glacial sequence (till) in the western 42 km^2 of the area (Koch, 2013). We only consider

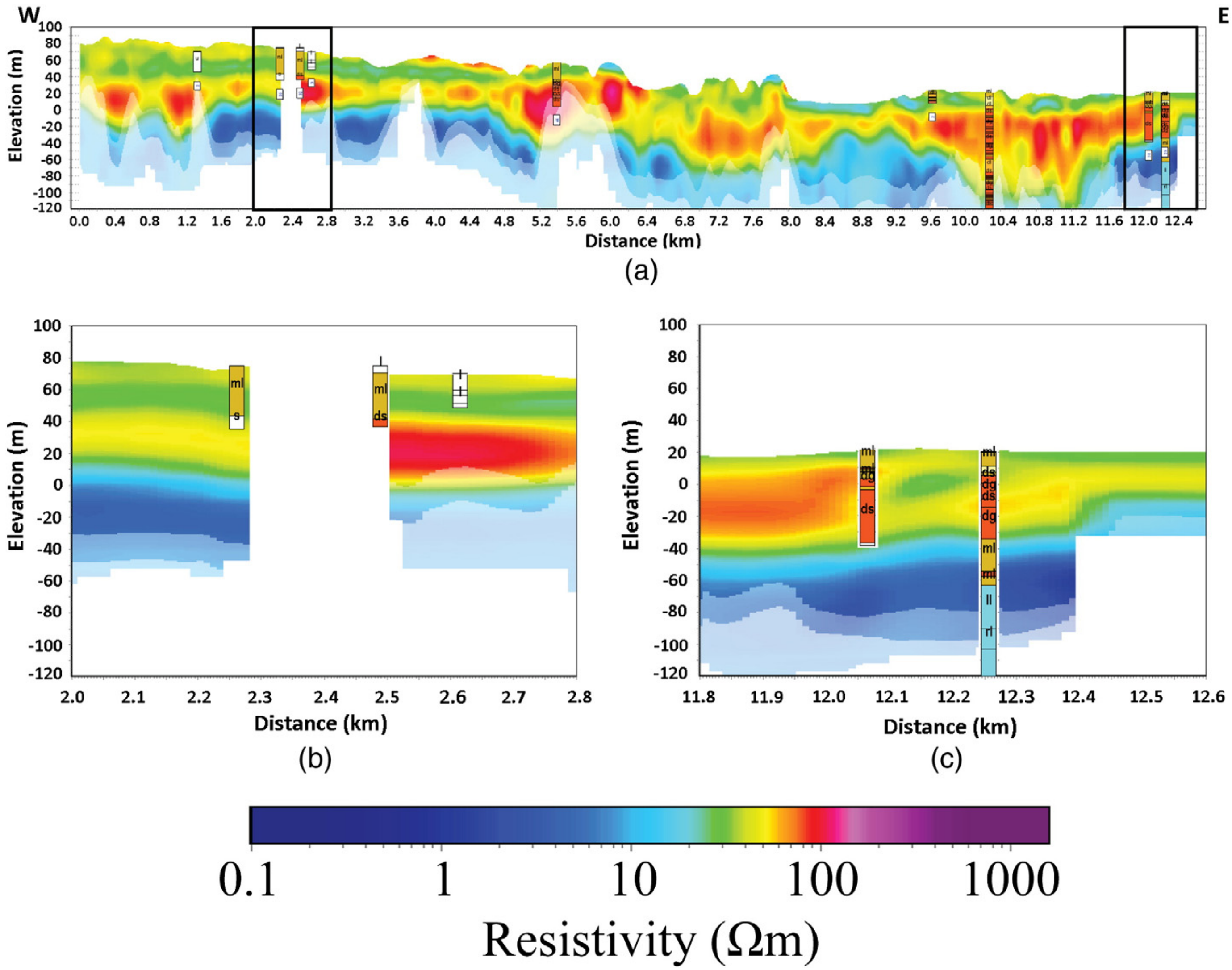

Fig. 5. SkyTEM results from the Norsminde catchment: (a) resistivity section of the profile drawn as a black line on map of Fig. 5 with borehole data; (b) zoom on the West part of the cross-section; (c) zoom on the East part of the cross-section. Borehole legend: dg = glacial gravel, s = sand, ds = diluvial sand, l = clay, ml = moraine clay, ll = plastic clay and rl = Eocene clay. All displayed boreholes are located within less than 50 m from the profile.

a binary system, namely sand and clay. The geostatistical properties in this area are inferred from both borehole data (vertical transition probabilities) and geophysical data (horizontal transition probabilities). The TPRoGS realisations are conditioned against both borehole and geophysical data. The conditioning probabilities for the borehole data range from 100% (hard conditioning) for the best quality boreholes to 85% for the used boreholes with the poorest quality, while the data from boreholes categorised as unreliable were not used.

To derive the conditioning probabilities for the geophysical data an analysis has been made of the relationship between probability of sand/clay seen in the best quality boreholes and resistivities in the nearest geophysical sounding. The result (Fig. 6) shows that resistivities less than 40 Ωm have a sand probability of less than 40%, while resistivities larger than 60 Ωm have sand probabilities of more than 70%.

The grid size for the TProGS simulations is 20 × 20 × 2 m. Examples of TProGS simulated geologies are shown in Fig. 7.

5.3. Hydrological modelling

A hydrological model based on the Mike SHE code is established for the Norsminde area with a 100 m grid and 2 m vertical resolution of the saturated zone. By introducing 10 different geological realisations simulated by TProGS and keeping all other data (unsaturated zone, river system, climate data, etc.) identical, 10 different hydrological models are generated. For each of the models the 10 most sensitive parameters are estimated by inverse modelling against observed data of hydraulic heads and river discharges for the period 2000–2003 using 1995–1999 as warm up period. The 10 calibrated models will be used for particle tracking. Fig. 8, showing results from a previous study in another catchment, illustrates the type of output that may be expected from such particle tracking modelling.

6. Discussion

6.1. Nitrate reduction in aquifer systems

While many studies have been conducted on nitrate transport and transformation processes in aquifer systems (Appelo and Postma, 1993; Welch et al., 2011), we are only aware of very few attempts to quantify aquifer nitrate reduction at catchment scale using spatially distributed groundwater models (Styczen and Storm, 1993b; Conan et al., 2003; Hansen et al., 2009). Transformation of nitrate in groundwater is generally a rapid process and hence the nitrate degradation at point scale is controlled by mass transport (Appelo and Postma, 1993). Several studies show that the distribution of nitrate is restricted to the

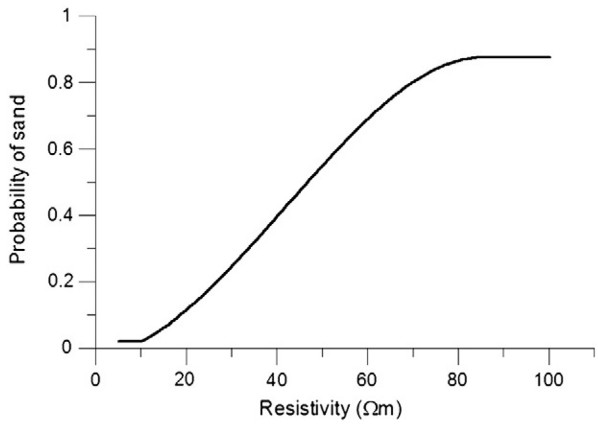

Fig. 6. Relationship between resistivity of SkyTEM soundings and probability of sand/clay in the Norsminde area for the best quality boreholes.

oxidized zone (Ernstsen, 1996) and that nitrate reduction often happens near the redox interface between the oxidized and the reduced zone (Ernstsen et al., 1998). We have therefore adopted the concept of instantly occurring nitrate reduction, when nitrate flows below the redox interface, as opposed to e.g. a first order process used by Conan et al. (2003). As flow paths in aquifer systems are known to be highly dependent on the geological conceptualization (Højberg and Refsgaard, 2005; Troldborg et al., 2007) geological uncertainties are likely to significantly affect where in the aquifer system the nitrate reduction actually takes place.

A major novelty in our approach lies in the combination of the different techniques (geophysics, stochastic geological modelling, hydrological modelling, uncertainty and scaling analyses) to assess both the location of the nitrate reduction within a catchment and the associated prediction uncertainty. In addition some of the applied techniques comprise novelties as described below.

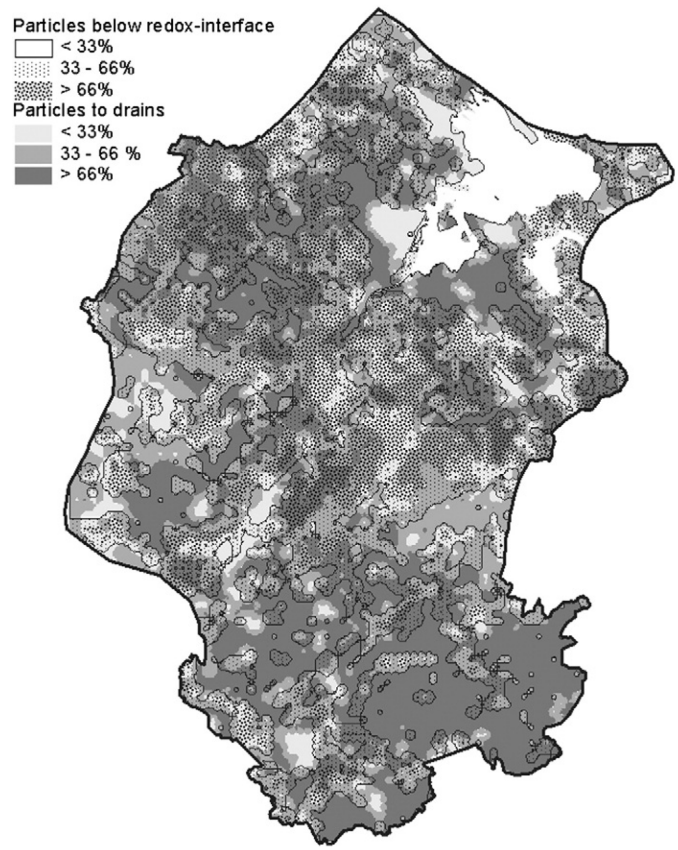

Fig. 8. Fractions of particles (i) that are transported below the redox interface and (ii) that are transported to the river via drains. Example for the Odense Fjord catchment (Hansen et al., 2009).

6.2. Airborne geophysics

High resolution geological data are prerequisites to enable detailed simulations of flow pathlines in aquifer systems that are required to delineate robust/vulnerable areas with high/low nitrate reduction. As such detailed geological information in practice can by far not be obtained from borehole data alone, geophysical data are therefore necessary (Thomsen et al., 2004; Jørgensen et al., 2012). Recent advances in airborne geophysics have made it possible in practice to map large areas by e.g. the SkyTEM method (Refsgaard et al., 2010b). The innovation in the new Mini-SkyTEM system developed here lies in a significantly improved spatial resolution down to 30–50 m horizontally and 2 m vertically in the upper 30 m obtained by combined hardware and software developments. The very early times data observed and interpreted with this system (<10 μs) bring the helicopter-borne transient EM system SkyTEM to a degree of resolution usually only achieved with frequency AEM systems but without the inherited problems with data calibration of frequency domain data (Ley-Cooper et al., 2006). Furthermore, the Mini-SkyTEM system maintains a better depth of investigation compared to what can be obtained for frequency AEM systems.

6.3. Stochastic geological modelling

Stochastic simulations of lithological units have been carried out by various indicator geostatistical tools such as TProGS (Carle et al., 1998) using transition probabilities, conditional simulation and quenching and SGEMS (Strebelle, 2002) using multipoint statistics and training images. What makes our study unique is that we have geophysical data to soft conditioning in all model grids.

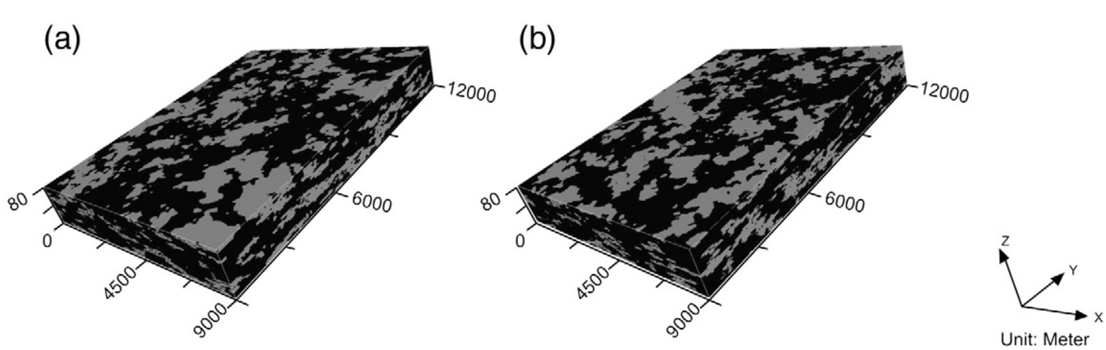

Fig. 7. Examples of two TProGS realisations from the Norsminde area. The dark and light colours correspond to clay and sand respectively.

The main reason for selecting TProGS was that it allows the use of borehole data to characterise the vertical resolution of geological units and at the same time using geophysical data to soft conditioning. As the vertical resolution (foot print) of the geophysical data is larger than the thickness of some sand lenses observed in boreholes, it would not be possible to reproduce such thin sand lenses if the geophysical data were used as training image as required with SGEMS. By utilising the vertical transitional probability characteristics from borehole data, we expect that our TProGS approach more accurately will be able to reproduce the sand lense patterns.

The conditioning probability for the SkyTEM data (Fig. 6) is based on the same idea as in Gunnink and Siemon (2009). This method lumps uncertainty from many sources into one curve relating the resistivity to the probability for finding sand/clay. The key uncertainties include: (i) inaccurate borehole descriptions; (ii) uncertainties on the resistivities due to geophysics instruments, field measurements and processing (inversion); (iii) lack of unique relationship between resistivity and lithology (sand/clay); and (iv) different spatial resolutions and hence different support scales for borehole data and geophysical data.

6.4. Drainage modelling

The flow paths in glacial till catchments in Denmark are significantly affected by tile drains, which have been constructed in most agricultural land in these catchments. In order to assess the amount of nitrate reduced in the aquifer system, it is important to be able to simulate drain water flows and hence the split of horizontal drain flows versus vertical groundwater recharge. Experience with simulation of drain flow indicates that models are generally not very good at predicting drain flows if they have not been calibrated specifically against the respective drain flows. This lack of performance may have several explanations such as (i) lack of local scale geological description (Hansen et al., 2013); (ii) lack of maintenance of the drains (van der Velde et al., 2010); or simply that (iii) the groundwater modelling concepts of simulating drain runoff as linearly proportional to the hydraulic head above a certain threshold (drain depth) over the entire model grid is not a suitable approximation for small drain catchments. We will investigate this by detailed modelling studies using the HydroGeoSphere (Therrien et al., 2008) testing different drainage modelling concepts such as representing drains by line elements or by preferential flow properties.

6.5. Scale of potential predictability — the RES concept

Distributed hydrological models can make predictions at grid scale, i.e. at much smaller scale than the full catchment. However, previous studies suggest that distributed models in general do not have predictive capability at scales smaller than the scale for which they have been calibrated (Refsgaard, 1997). Hansen et al. (2013) tried to simulate runoff in drain pipes from five 2–4 ha drain catchments within the Lillebæk catchment by a MIKE SHE based hydrological model calibrated against groundwater heads from 13 observation wells and discharge data from two river gauging station (Hansen et al., 2013). They found that the model was neither able to predict the differences in runoff between the five discharge stations nor the differences in amplitude of annual head fluctuations among the 13 observation wells. A possible explanation for this lack of local scale performance might be that the geological model was based on data from few geological wells (no geophysical data were included) and hence local scale hydrogeological heterogeneities were not well described.

We are characterising the uncertainty of the model predictions due to geological uncertainty by the standard deviation between predictions of different models based on different geological realisations. By assessing this uncertainty for different spatial scales of aggregations (e.g. 1, 2, 4, 8, 16 etc. model grids) we derive a relationship between prediction uncertainty and scale. The scale of potential model predictability (RES) is then equivalent to the spatial scale at which the prediction uncertainty is equal to a given acceptable level of uncertainty (Fig. 1).

The representative elementary area (REA) concept, which is very similar to our new RES concept, has several applications in rainfall runoff modelling (Wood et al., 1988; Beven, 1995), where it is typically related to uncertainty in precipitation and land use. He et al. (2011) used the concept to study the effects of precipitation uncertainty using radar on simulations of a coupled groundwater-surface water model. In an analysis of different domain sizes and grid sizes of two regional climate models Rasmussen et al. (2012) used the same concept (denoted as inter-model standard deviation length scale) for assessing the scale of potential model capability to predict precipitation. To our knowledge, however, this concept has, except for He et al. (2011), not been used in groundwater modelling.

As the RES is conditioned on a given model, it will only have predictive capability with the indicated uncertainty if the model in all other respects is correct. Thus, the RES is the theoretically minimum scale a model with a given geological conceptualisation can obtain a predictive accuracy corresponding to the given acceptable accuracy. In principle other uncertain factors could be addressed within the framework. Other key uncertainties in this respect that should be assessed in future studies include (i) spatial heterogeneity of hydraulic conductivities within sand and clay units; (ii) the depth to redox interface; and (iii) the conceptualisation of runoff in tile drains.

6.6. Water management perspectives

The goals of the work are to help target measures, in particular their spatial location, so that the nitrate loss can be reduced, and to assess the uncertainty of the nitrate reduction as a function of the spatial scale at which it is assessed. The developed framework and techniques has the potential for adopting a more cost effective measure to mitigate nitrate load from agricultural areas, namely to exploit the spatial differences in nature's own capacity to reduce nitrate in the aquifer system. This requires identification of robust areas, where nitrate leaching through the root zone is reduced in the saturated zone before reaching the streams, and vulnerable areas, where no subsurface reductions takes place, and imposing regulations /restrictions only on the vulnerable areas. Such a measure is only relevant in areas where a substantial part of the nitrate leached from the root zone is reduced in the aquifer system.

One prerequisite for implementing such a measure is that detailed spatial geological data are available. The results obtained with the new MiniSkyTEM airborne transient electromagnetic system are very encouraging in this respect. With this very fine spatial resolution and the ability to map large areas for a relatively modest cost, it provides a unique potential for developing more detailed geological and hydrological models to support delineating robust/vulnerable areas at a relatively small spatial scale.

As the regulations on vulnerable areas may be quite dramatic in terms of restricting the possibilities for having economically feasible agriculture, and hence may have both economical and personal/societal impacts, it is required that robust and vulnerable areas can be identified with sufficient accuracy. The framework and tools have been developed with the specific purpose of assessing the prediction uncertainty of delineating such areas, including identifying the smallest scale (RES) for which the accuracy is satisfactory to allow use of such a measure. If the results show that RES is in the order of a km^2 or less it has a great potential for use in practical water management. If, on the other hand, the results show that RES is in the order of 10 km^2 or more, it will not be very useful in practice in a Danish context.

Preliminary analysis indicate that site specific regulation aimed at achieving the current nitrogen loss would allow 70% of all farmers to apply more nitrogen on selected fields, whereas 30% would have to apply less. This requires that the farmers follow the instructions and apply nitrogen, where it is allowed in a field. However, there will be a strong economic incentive to move the nitrogen from fields with high N-quotas to fields with low N-quotas within the farm. This would reduce the environmental effect and would then again require stricter N-quotas to achieve the same environmental target.

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