

Testing the application and limitation of stochastic simulations to predict the lithology of glacial and fluvial deposits in Central Glasgow, UK.

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ABSTRACT

Glacigenic and fluvial deposits of variable lithological composition underlie many major cities in Europe and North America. Traditional geological mapping and 3D modelling techniques rarely capture this complexity as they use lithostratigraphic designations which are commonly based on genesis and age rather than lithological compositions.

In urban areas, thousands of boreholes have been, and continue to be, drilled to facilitate the planning, design and construction of buildings and infrastructure. While these data may provide the basis for geological maps and 3D models based on lithological interpretation, they are too numerous for manual correlation to be undertaken efficiently. In this paper we explore the application of largely automated stochastic modelling techniques to develop predictive lithology models for glacial and fluvial deposits in the city of Glasgow, UK. These techniques are commonly used to assess facies variation in oilfield models and are applied here in an urban setting using over 4000 borehole records.

Predictions derived from these methods have been evaluated by removing control data and re-running the simulations. We demonstrate a moderate improvement in the prediction of lithology when using a lithologically-derived stochastic model compared with a conventionally interpolated

lithostratigraphic model. It is possible to report uncertainty within the resulting models, either with probability maps or through a suite of plausible simulations of the lithologies across the study region.

1. Introduction

The growth and decay of high- and mid-latitude Pleistocene ice sheets has left 8% of the Earth's land surface, including one third of Europe and a quarter of North America, covered by glacial and fluvial deposits (Ehlers and Gibbard, 2004a, 2004b). These deposits underlie many major cities and much of their associated infrastructure networks, and exert a significant influence on the groundwater system. Increasing urban development, and its demands (e.g. suitable foundation conditions, the need for waste storage, contaminant migration, drainage re-routing) requires that information about subsurface glacial deposits, which are often highly lithologically variable across short distances, is available for those involved in planning and construction (Campbell et al., 2010). A key challenge for the three-dimensional (3D) geological modelling community is therefore to represent these subsurface deposits in appropriate ways across large, city-wide areas (Culshaw, 2005; MacCormack et al., 2005; Kessler et al., 2009).

In Glasgow, west central Scotland (Figure 1), the British Geological Survey (BGS), in partnership with Glasgow City Council and other local authorities, have used extensive borehole datasets to develop and successfully apply a suite of 3D Quaternary lithostratigraphic models (Merritt et al., 2007; Campbell et al., 2010) (Figure 2). A key strength of lithostratigraphic modelling is that it brings together the expertise of geologists and known geological relationships, enabling a geologically realistic representation, even where subsurface data are lacking (Kessler et al., 2009). However, owing to the complex and heterogeneous nature of glacial deposits (Hambrey, 1994; Meriano and Eyles, 2009; Benn and Evans, 2010), lithostratigraphic modelling may not always represent the full subsurface variability that is of direct relevance to end-users, such as ground engineers or

groundwater modellers. Furthermore, this approach is time-consuming. For example, extending the same detailed lithostratigraphic modelling methodology that was used for Glasgow, to all UK cities would be highly protracted engaging considerable resources over a number of decades – too long to be of use to many current and planned urban redevelopment schemes. In this paper we explore a largely-automated facies-based stochastic modelling approach to investigate lithological variations within glacial and postglacial fluvial and marine deposits. Stochastic models can be used to produce multiple realisations of the lithological variation across the model domain. Rather than producing a single solution, this allows a wide-range of realisations. These multiple solutions can be used to generate lithology probability maps, which capture the lithological variation. In this way, stochastic simulation, as opposed to interpolation techniques, captures not only the most likely lithology at a given location, but also uncertainty within the simulations. This may be particularly beneficial if the lithological simulation is to be subsequently used to model the distribution of hydraulic or geotechnical parameters, as it allows for different scenarios to be modelled. From a ground engineering perspective, it is also useful because it can highlight areas in the model that are data poor and require further ground investigation.

Stochastic geological modelling owes its origins to the hydrocarbons industry, where it is widely used to characterise and simulate reservoir heterogeneity (Wach et al., 2004; Yarus and Chambers, 2006, Falivene et al., 2007). Rather than producing sharp boundaries between units, it allows lithologies to grade into each other which better captures the inter-fingered nature of heterolithic deposits. Central Glasgow is well suited for this type of approach, as more than 4000 geotechnical and lithological borehole logs are available to condition the simulation.

Our motivation is to test whether a lithology-based stochastic modelling approach can produce a geologically valid representation of subsurface lithological variation in a complex depositional environment affected by glaciation – typical of the Quaternary geology under many cities in North America and Northern Europe.

2. Research Aims

Few studies have attempted to apply stochastic modelling to the lithology of terrestrial Quaternary deposits (c.f. Comunian et al., 2011). However, the technique has been demonstrated to be a valid and potentially successful approach in fluvio-deltaic sediments of the Netherlands (Stafleu et al., 2011). To our knowledge, the technique remains untested in a complex formerly glaciated environment affected by a combination of ice sheet oscillations, relative sea level changes and post glacial fluvial processes, such as occurred in Glasgow (Browne and McMillan, 1989; Finlayson et al., 2010). In this paper, and for the first time in the UK, we developed and tested a stochastic approach to modelling the distribution of complex Quaternary deposits at a city-wide scale. Our principal research goals are listed below.

1. Apply facies-based stochastic modelling methodologies to simulate the distribution of Quaternary deposits in central Glasgow.
2. Describe the basic characteristics of the model, and highlight the assumptions and the limitations of using a stochastic modelling approach.
3. Compare two different stochastic models with each other and the lithostratigraphic model by: i) removing a portion of the input boreholes and re-running the simulation to look at internal variance in the model (Hass and Formery 2002, Scheidt and Caers, 2010); ii) Evaluation of the model was also done by testing it against boreholes that were not used in the stochastic modelling (Browne and McMillan, 1989; Hall et al., 1998).
4. Offer recommendations as to the future applicability of the technique to other cities built in formerly glaciated environments.

3. Geological Setting

The Glasgow conurbation, Scotland's most densely populated area, is located alongside the River Clyde in west central Scotland (Figure 1). In the 19th and early 20th centuries, much activity in Glasgow (and surrounding areas) was based around mining and heavy industry (Browne et al., 1986). Subsequent industrial decline has left significant areas of dereliction, which have been the targets of a major 25-year regeneration plan (Campbell et al., 2010). It is recognised that future sustainable development in Glasgow requires an understanding of the nature and distribution of subsurface Quaternary deposits (Glasgow City Council, 2011). The present study focuses on a 100 km² area in central Glasgow (55.813°N–55.903°N; 4.157°W–4.319°W) (Figure 1).

The Clyde Basin is thought to have been glaciated at least five times in the last 0.5 Ma (Lee et al., 2012), most recently during the Main Late Devensian glaciation, when ice advanced into the basin sometime after 35 thousand years BP (Brown et al., 2007; Jacobi et al., 2009). Glacier ice had retreated from the Glasgow area by ~15 thousand years BP, at which time the late glacial relative sea level had risen locally to almost 40 m above current sea level (Peacock, 2003). Relative sea level fall during the Holocene resulted in a series of raised estuarine flats around the Glasgow area at progressively lower elevations from ~12 m to ~3 m above current sea level. A full description of events during and following the last glacial cycle in Glasgow, and associated lithostratigraphic variations is described elsewhere (Browne and McMillan, 1989; Finlayson et al., 2010; Finlayson, 2012).

The key units relevant to the present study are summarised in Table 1 and Figure 2. The *Wilderness Till Formation* comprises a massive to locally stratified sandy silty clay diamicton. It has been noted to include rare bands of sand and laminated clay; these are generally < 10 cm thick, but one temporary section has also revealed metre-scale till interbeds (Browne and McMillan, 1989). These may be the result of glaciotectonic thrusting and hydrofracturing near the former ice margin as it advanced into the Clyde basin (Finlayson, 2012). The *Wilderness Till Formation* probably rests on

bedrock across much of the study area. However, in bedrock depressions in the northern parts of the study area, it may also overlie buried glaciofluvial sands and gravels, buried glaciolacustrine clays and a lower till belonging respectively to the *Cadder Sand and Gravel Formation*, the *Broomhill Clay Formation* and *Baillieston Till Formation*. The *Wilderness Till Formation* is overlain by the *Bridgeton Sand Formation*. It generally comprises an upward-fining sequence of medium- to fine-grained sand, with some gravel beds and rare, isolated stones (< 10 cm). The *Bridgeton Sand Formation* is thought to have been deposited in the central Glasgow area as subaqueous (probably glaciomarine) outwash fans at the margin of *in situ* decaying ice (Figure 2, Section 1 and 2). The *Bridgeton Sand Member* is overlain by the *Paisley Clay Member* of the *Clyde Clay Formation*, which generally comprises laminated silts and clays with isolated bands of sand and dropstones (Figure 2, Section 1 and 2). The *Paisley Clay Member* was laid down in a glaciomarine environment, shortly after complete ice decay in Glasgow, when relative sea level approached 40 m above current sea level. Along the margins of the River Clyde, the *Paisley Clay Member* may be overlain by the *Gourock Sand Member* (Figure 2, Section 1 and 2), which generally comprises fine- to coarse-grained sand, but may also include clay, silt and gravel beds. In the study area, these deposits are thought to have been deposited in a shallow, fluviually influenced, estuarine environment, when relative sea levels were 3 m – 12 m higher than today.

These lithostratigraphic units can be broadly divided into two separate sedimentological facies, glacial and post-glacial. The glacial facies includes the *Wilderness Till Formation*, *Cadder Sand and Gravel Formation*, the *Broomhill Clay Formation* and *Baillieston Till*. The post-glacial facies includes all units overlying the *Wilderness Till Formation* (including the *Bridgeton Sand Formation*, *Paisley Clay Member*, *Gourock Sand Member*) that were formed following ice retreat and during subsequent sea-level variations. The boundary between these two facies is the top of the *Wilderness Till Formation* which represents a disconformable sequence boundary. There is no interfingering between these two facies, although lithologies that belong to a single facies may interfinger.

As described previously, all lithostratigraphic units are highly heterolithic. If a single lithology is assumed for each lithostratigraphic unit based on the major component in the published lithostratigraphic description (Browne & McMillan, 1989, Table 1), there is only a 54% match when compared against the borehole data used in this study (see Section 4.1 for description of boreholes). For individual lithostratigraphic units this figure varies between 3% and 68% (Table 1). This suggests that a simple lithostratigraphic approach can only predict the lithologies in a borehole about half the time, and that the minor lithologies occurring within the lithostratigraphic units represent a significant proportion of the total volume of these units.

4. Materials and Methodology

The methodology used in this work combines: (i) borehole data collected from site investigations and other geotechnical applications, which were prepared for input into GOCAD® software; (ii) the creation of stochastic models in GOCAD® software, and (iii) the comparison of this model against previously published data and analysis of the results.

4.1. Input data

The dataset (Figure 3) includes the geological logs of 4391 geotechnical boreholes, collected over several decades for a variety of purposes by different ground investigation contractors. These borehole logs are digitally stored in a database and are recalled as tab-separated ASCII files for use in modelling workflows (see Kessler et al., 2009 for more details). The boreholes have a maximum depth of 79 m and a minimum depth of 3m, with a median depth of 6 m. Collectively, the dataset includes 21320 individual descriptions of the lithology at particular locations and depths that were described in accordance with British Standard BS930:1990 (British Standards Institution, 1999). BS930 standard descriptions systematically describe the relative density or consistency, structure, colour, size, and relative proportions of composite particles. Within the dataset, each record had

been assigned a code by BGS, based on the borehole log description; this code represents the major lithology at that position as described in the textural lithological description (e.g. sand and gravel), using an internal BGS classification scheme defined by Cooper et al. (2006). Because the original core from these 4391 geotechnical boreholes no longer exists it is impossible to do any independent validation of the borehole log descriptions, a situation that is common in all urban settings. Initial processing of the data indicated that 185 different lithological codes have been used to describe the Quaternary deposits recovered from these boreholes, which is too many to include in a modelling exercise. Further examination of the data showed that of these 185 codes, 21 of them account for over 87% of the records in the study area. Accordingly, these 21 codes were simplified and automatically assigned into nine main categories, based on the dominant observed lithology (or lithologies) and consistency that were described in each record. The nine categories are: 'organic', 'soft clay', 'soft clay and sand', 'stiff clay diamicton', 'silt,' 'silt and sand', 'sand', 'sand and gravel', 'gravel.' Records with lithological codes not ascribed to the 21 lithology codes (approximately 2,500 lithology descriptions) were manually assigned to a category based on available descriptive information.

Particle size distribution data were available for 3196 of the lithology records, and were used to compare and validate the nine categories (Williams and Dobbs, 2012). This analysis revealed that the 'clay and sand' and 'clay' categories have similar particle size distributions, and so the two categories were combined into a 'soft clay' category. This was also true of the 'silt and sand' and 'sand' categories, as well as the 'sand and gravel', and 'gravel' categories, so these pairs were combined respectively into a 'silt' and 'sand and gravel' category. The 'stiff clay diamicton' category was defined using criteria of lithological description and consistency. The 'stiff clay diamicton' category has a consistency of 'firm to very stiff', as compared to the 'soft clay' category, which has a consistency of 'soft to firm'. This difference reflects the fact that, in Glasgow, clay-diamicton was

generally, though not exclusively, deposited beneath glaciers as till, and has been shown to have a significantly stiffer consistency than the post-glacial clays, caused by ice compaction rather than other factors such as depth from surface and water content (Entwistle et al 2008). The distinction of 'stiff clay diamicton' and 'soft clay' also addresses a specific geotechnical problem relevant to the Glasgow area. The end result of reclassification using textural analysis of borehole log descriptions and particle size analysis was to reduce the number of lithological categories to six : 'organic', 'soft clay', 'stiff clay diamicton', 'silt', 'sand', and 'sand and gravel'.

4.2. Three-dimensional model construction

The base of the model domain was defined by using a surface representing rock-head (the boundary between the bedrock deposits and overlying superficial deposits) that was taken from the existing lithostratigraphic model of the study area (Figure 2, Merritt et al., 2007). The top (or capping) surface was based on the NEXTMap™ Britain digital elevation model (© Intermap technologies). However, man-made deposits at the land surface were excluded from the modelling domain, thereby incorporating the base of the artificial ground layer, which had been identified during earlier lithostratigraphic modelling (Figure 2, Merritt et al., 2007), into the capping surface. Artificial ground was excluded because it does not conform with the glacial and postglacial sediments and was too variable in description to be able to interpolate between points. Stochastic modelling could be applied to modelling the variability of artificial ground. However, it would require an understanding of the factors that control the occurrence of different manmade deposits such as positions of former industrial sites and remediation and thus falls outside the scope of this study. The surfaces representing rock-head and the digital elevation model, modified to remove artificial ground, were imported into GOCAD® and used to define the base and top of the model domain. The modelling volume is 10 km x 10 km wide and 80 m thick, and comprises a regular grid of discrete cellular volumes, each 50 m x 50 m x 0.5 m in size. The vertical thickness of the grid was defined by being half the median thickness of the lithological unit observed in the borehole data (median 1 m, min 0.1

m, max 34 m). The horizontal grid resolution was defined as a compromise between ensuring reasonable computational performance and the city-wide scale of the modelling program. This grid was subdivided into two separate regions, representing glacial and post-glacial facies, using a surface from the existing lithostratigraphic model that represents the top of the Wilderness Till (Figure 2, Merritt et al., 2007). This was done as the top of the Wilderness Till defines the sequence boundary between these two facies.

The borehole information were imported to GOCAD® with each of the six lithological categories attributed as a discrete property. Lithologies were then stochastically modelled (simulated) across the grid using Indicator Kriging (IK) and Sequential Indicator Simulation (SIS) methods, conditioned to the input borehole dataset (Deutsch and Journel, 1992). Indicator Kriging (IK) takes the input borehole data and, where the borehole is present in the grid, assigns a value of one where that lithology is present while assigning all other lithologies a value of zero. It then interpolates the results obtained for all indicator variables (lithology) for each cell in the grid and the lithology to obtain maps of the probabilities of each lithology occurring at that cell. A map of the most likely lithology in each cell can be inferred from the probability maps for the individual lithologies (Falivene et al. 2007).

Sequential Indicator Simulation (SIS) works in a similar way to IK, but begins at a random cell in the grid. IK is used to determine the probability of each lithology occurring at that cell. The realised lithology for the cell is selected at random according to these probabilities. It then moves randomly through the remaining grid cells and performs the same calculation, using the values realised in previous cells as conditioning data for subsequent cells (Falivene et al., 2007). By this method, SIS takes account of both the input data and the other values in the grid, which produces more

gradational contacts between different lithologies. The results of indicator simulations such as SIS are dependent on a randomly selected seed number, that determines the cell in which the algorithm begins and the random selection of the lithology in each cell. Use of different initial seed numbers results in different realisations of the same property, generating multiple realisations and enabling an understanding of the variability of the modelling results and of the inherent uncertainty involved. The SIS algorithm was used to produce 500 realisations using different seed numbers, and therefore the probability that any one lithology will occur at any specified site in the grid could be estimated. Whilst the precision of these estimated probabilities could be increased by increasing the number of simulated realisations, this would have required more computation time. For example, if a particular lithology occurs in a particular cell with probability 0.3 and we treat the realisations in that cell as a set of independent binomial trials, then the 500 realisations would lead to a standard error of 0.02 in estimating the probability of occurrence. We judge this level of precision to be sufficient.

The probability of each lithology occurring at any particular cell can also be extracted from the IK methodology without the need for the use of SIS. However, the advantage of SIS is that within each realisation it is possible to see the shapes of lithological bodies that are likely to occur (both horizontally and vertically). This information is lost in a simple probability model since it is not clear to what extent the lithology in one cell is correlated with the lithologies in adjacent cells.

The IK and SIS algorithms require three inputs. The first is the set of conditioning observations of lithology. These were derived from the borehole data. However, the interpolation algorithms require that the observations are expressed at the same spatial scale as the cells within which the lithology will be modelled. Therefore the borehole data were up-scaled to 50 m x 50 m x 0.5 m cells. There are two options as to how to do this in GOCAD®: 1) by calculating which of the borehole observed

lithologies has the largest proportion in each cell intersected by boreholes in the grid; 2) calculating which of the lithologies was closest to the centre of each cell in the grid intersected by a borehole. We selected the first option since we required that the observations were representative of the entire volume rather than just the centre. It is clear that the up-scaling process removes some of the fine-scale variability seen in the original input data, which will be detrimental if the model results are to be explored at the fine-scale. As the individual grid cells are 50 m x 50 m x 0.5 m this should be seen as the maximum scalar resolution of the model. A finer resolution grid would be preferable; however, the grid size was limited by the computational power available to this study.

The second set of inputs for the modelling algorithms is the proportion of each separate lithology throughout the study region (the global proportions of each lithology) (Figure 4). The IK methodology assumes that in a cell that is a long distance from any conditioning data that the modelled probability of a particular lithology will be equal to the global proportions of this lithology. In cells close to conditioning data the modelled probability will be largely controlled by these conditioning data. We determine the global proportions from the observed lithologies scaled up to the cell scale. It should be noted that if the boreholes are clustered then certain areas of the study region will be over-represented and the proportion of boreholes with a particular lithology will be a biased estimate of the proportion of the study region with this lithology. The up-scaling of input observations will remove the effect of clustering at the within-cell scale. Thus the influence of the effects of clustered data will be largely confined to cells that are distant from the conditioning data.

The final inputs to the IK and SIS methodologies are models, referred to as variograms, of the spatial dependence of the data (Cressie, 1993). These variograms quantify the extent to which the probability of observing the same lithology at two different sites increases as the separation

between these sites decreases. GOCAD® calculates point estimates of the variograms for each lithology. These point estimates consist of plots of half the average squared difference between the values of the indicator variables at a pair of locations against the distance separating the pair of locations. The user then fits a different parametric variogram model to the point estimates for each lithology. One parameter of each variogram describes the range of spatial correlation. Beyond this separation distance the observed lithologies can be considered to be independent of each other. In this way, varying the variogram range parameters between different lithologies allows for some control over the shapes of the stochastically generated litho-bodies (Table 2). Exploratory analysis of the point estimates of the variogram suggested that the spatial variance of the 'stiff clay diamicton' exhibits an isotropic spatial dependence, which is different from the fluvially derived 'soft clay' which exhibits a stronger degree of spatial dependence in the mean direction of sediment transport along the present Clyde Valley. The remaining lithologies were assigned a common isotropic variogram which has a shorter variogram range than the 'soft clay' category, because there was little difference in the point variogram estimates for each category. Vertical range values for all categories were set to 1 m, which is the median thickness of the lithology observed in the borehole data.

In common with any modelling methodology, this approach makes a number of assumptions about the nature of the spatial variation of the lithological categories. For instance, it assumes that the variograms and global proportions of each lithology have been reliably estimated and that the same variogram models apply throughout the study region. Given the large number of data used to calculate our models we anticipate that deviations from these assumptions will have little effect on the final outputs. The effects are likely to be largest at sites that are distant from any conditioning data, where the uncertainty about the lithology is largest.

4.3. Validation Tests

It is not possible to directly compare stochastic models and traditional lithostratigraphic maps or models because the results of a stochastic model are best displayed in terms of the relative probabilities of the presence of a certain lithology rather than as a definitive map.

Therefore, the predictive ability of both the IK and SIS models was investigated by testing them against two BGS boreholes that contributed to defining the published lithostratigraphy of the area (Browne and McMillan, 1989). Also, the stochastic models were tested by randomly excluding 50% of the input boreholes from the conditioning data, re-running the simulation and then comparing the result to the 50% boreholes that were removed. This technique is commonly used in the oil industry and is sometimes referred to as bootstrapping (Haas and Formery, 2002; Scheidt and Caers, 2010). We used these bootstrapping tests to quantify the reliability of our predictions of lithology and to confirm whether our spatial modelling methodology performs better than simpler non-spatial models.

5. Results of simulations

5.1. SIS and IK results

The modelling domain contains $\sim 9.5 \times 10^5$ individual cells. The SIS was run 500 times using different seed numbers. From these different realisations it is possible to calculate the number of times that any given lithology occurs at any one cell in the model. This can be expressed as a range of probabilities, from 0 (never occurs) to 1 (always present), that any of the lithologies occurs in any given cell over the 500 simulations (see Figures 5, 6 and 7). Those cells containing conditioning data (boreholes) will return a probability of 1. The simulations can be used to generate a 3D map of the most probable lithology at every point in the study region. In Figure 5 (a) and (b), the IK and SIS predictions of the most likely lithology at each surface location are compared. The maps are very

similar except isolated predictions of soft clay occur in the SIS map that are not evident in the IK map. These clay features tend to occur in areas where borehole data are sparse and we expect they are an artefact of the simulation method, occurring as a consequence of the estimated probabilities of clay and sand being very similar in these areas since the global proportion of clay is only slightly less than the global proportion of sand (Figure 4).

We do not recommend that these maps of most likely lithology are viewed in isolation since they say nothing about the uncertainty in the model. The magnitude of this uncertainty will vary across the study region and it will be smallest in regions where the density of boreholes is highest. The magnitude of the uncertainty at a site is reflected in probability maps shown in Figure 5 (c). Similar probability maps could also be produced by using IK. These maps fully reflect our uncertain knowledge of the lithology in each cell but they say nothing about how the lithology in a cell is correlated to the lithologies in adjacent cells and hence the shape of lithological bodies that are likely to occur. This information is contained in the individual realisations of the SIS.

Comparing the IK and SIS most frequently occurring models (Figure 5, 6 and 7) to the lithostratigraphic model (Figure 2), the broad geometries of the units appear to agree. For example, 'stiff clay diamicton' is preferentially distributed across the higher ground on either side of the Clyde Valley. Lithologies such as 'soft clay' and 'sand' are preferentially distributed on the low ground along the present Clyde Valley axis. However, there is disagreement with the lithostratigraphic model as to the extent of units such as the Paisley Clay if it is assumed to comprise only clay. Both the IK and SIS suggest that along the valley axis the clays are cut by areas of 'sand' or 'silt' (Figures 2 and 6).

Both techniques suggest that there is no visible lithological division between units such as the Gourock and Bridgeton Sand Members (Figure 2 and 6).

5.2. Validation tests

To test the predictive ability of both the IK and SIS, 50% of the boreholes were randomly excluded and the simulations re-run to compare the new models against the known removed values. To allow like-with-like comparison, the up-scaled boreholes were removed from the grid rather than the raw boreholes.

The IK results generated the observed lithology for the up-scaled boreholes that had been removed from the grid in 10695 cells out of 18019, meaning the IK methodology predicted the known lithology 59.35% of the time.

To test the SIS the most frequently occurring lithology per cell over all the 500 simulations was compared. This generated the correct answer for the up-scaled boreholes that had been removed from the grid in 10735 cells out of 18019, which meant the SIS simulation predicted the correct lithology 59.58% of the time. For comparison, had the predicted lithology been selected at random, the expected agreement would have been 15%. Had sand, generally the most abundant lithology, been predicted everywhere, the expected agreement would have been 30%.

However, the most frequently occurring lithology over the 500 simulations may not be the best way to assess the accuracy of the SIS simulation. This is because there may be only one simulation separating the most frequently occurring lithology and the next most frequently occurring lithology. Additionally, less frequently occurring lithologies (such as 'organic' and 'sand and gravel'), which have a major impact on ground conditions where they occur, tend to be under-represented if the most likely lithology is selected at each site. Although there may only be a relatively low probability that these lithologies may occur at any one specified site, they might occur a sizable number of times across a large study region. We therefore considered how well the modelled probabilities at each of the randomly removed boreholes reflected our uncertain knowledge of the observed

lithologies and whether our approach performed better than a non-spatial model. The non-spatial model assumes that the probability of a particular lithology occurring is the same everywhere in the study region. Also that it is equal to the proportion of the input data at the cell scale to realise this lithology throughout the study region. Using this model we find that the average probability of the observed lithology at the validation sites is 0.25. In contrast, the average probability according to our spatial model is 0.51, indicating that the SIS probability methodology leads to substantially more informative probabilistic models.

5.3 BGS Borehole Comparisons

The BGS Bridgeton and Broomhill Park boreholes contributed to the original development of a lithostratigraphy for the superficial deposits in the Glasgow area (Browne and McMillan, 1989; Hall et al., 1998 Figure 3). However, neither borehole was used as input data for the stochastic model. Therefore, these boreholes provide a useful test of the representativeness of the stochastic model at point localities. The Bridgeton and Broomhill Park boreholes are 80 m and 192 m respectively from the nearest conditioning boreholes.

Broadly both the IK and SIS models predict similar overall proportions of lithologies present in the Bridgeton Borehole (Figure 8). However, both models appear to underestimate the amount of clay present in the borehole. Both the IK and SIS models fail to accurately predict the depth of the major changes in lithology seen in the borehole. The individual lithology probabilities are slightly more predictive as there is an increased probability of (0.4–0.6) of the occurrence of 'sand and gravel' within 1 m of the vertical position of the sandy gravel of *Gourock Sand Member* seen in the borehole (Figure 8). However, the vertical thickness suggested by either the IK or SIS models is much greater than observed in the borehole. Equally there is an over prediction of the amount and thickness of

sand at this precise locality, which may be due to the fact that the model becomes homogenous with depth due to lack of data.

The comparison between the Broomhill Park Borehole and the stochastic model shows a similar result (Figure 9). The stochastic model predicts high probabilities of 'clay diamicton', which is the lithology most often seen in the *Wilderness Till Formation*, throughout the depth of the borehole. However, laminated clays of the Broomhill Clay Formation were observed in the lower eight metres of this borehole; although these were not captured by the stochastic modelling.

5.4 Investigating whether model accuracy varies with depth

The stochastic model broadly captured the observed composition of the Bridgeton and Broomhill Park boreholes. Given that lithology can vary over short distances it is unsurprising that some discrepancies between the observed and modelled lithology were evident. However, these discrepancies increased with depth in both boreholes. Therefore we looked further at the deletion tests to explore whether the model generally became less accurate with depth. The results from the deletion tests were plotted against depth from surface (Figure 10). This showed that although there is a decrease in accuracy with depth from surface across the model as a whole it only starts to show a prolonged decrease in accuracy below 32 metres from surface. Only 0.8% of the entire model is deeper than 32 metres from the surface.

6. Discussion

Our deletion tests have shown that our modelling methodologies are slightly more accurate at predicting the lithology within the cells containing boreholes than the lithostratigraphic model (assuming the dominant lithology is the only lithology present in each lithostratigraphic unit). The IK

and SIS methodologies predicted the actual lithology at 59.35% and 59.58% of the locations respectively in comparison to the 54% correct predictions from the lithostratigraphic model. However, it should be noted that the boreholes are clustered and these results do not necessarily reflect the reliability of the methodologies in areas where boreholes are sparse. However, borehole clustering is an inherent source of bias in both stochastic and lithostratigraphic models (see Merritt et al. 2007) as both approaches use the geotechnical boreholes as their main source of subsurface data. The deletion tests also confirm that our models are more accurate than simpler stochastic models that do not account for spatial correlation in the observed lithologies.

The clustering in the data can create problems in applying the IK and SIS methodologies. It can lead to biased estimates of the global proportion of each lithology (Deutsch and Journel, 2009). When producing a 3D lithological model, it would be ideal if the boreholes were evenly distributed across the study region (van Groenigen et al., 1999) but in reality boreholes are likely to be clustered in areas of specific interest. The biases in the global proportions of each lithology will have little effect on the lithological model where boreholes are plentiful but the modelled results in areas that are distant from boreholes should be treated with some caution (MacCormack & Eyles, 2012). The elevated uncertainty in regions where boreholes are sparse is also observed with the BGS boreholes (Figure 8 and 9) as they are only 80 m and 192 m away from the nearest control data and only predict the observed lithology in the broadest terms.

The comparison with the BGS boreholes (Figure 8 and 9) seems to indicate that the model can only accurately predict lithology to a depth of approximately 10 metres. However, when results from the deletion tests were plotted against depth from surface (Figure 10) there is no sustained decrease in accuracy of the model until below 32 metres below the surface. Given that lithology can vary over short distances it is unsurprising that some discrepancies between the observed and modelled lithology were evident. For a site-specific model a finer-scale grids would be more appropriate and

give a better correlation with individual boreholes. However, the grid size in the study was limited by computational power.

One important attribute of the IK and SIS methodologies is that they can calculate the uncertainty associated with the lithological model. Both approaches can express the probability of each lithology occurring in a particular cell and hence areas where the model is unreliable can be quickly identified. In addition the individual SIS realisations reflect the actual shapes of lithological bodies and their relationships that we might expect to occur (compare the IK and SIS models Figure 6–7).

Previous stochastic studies have recommended sub-dividing the model volume into lithostratigraphic packages prior to stochastic modelling, so that stratigraphically separated lithologies cannot interact (Comunian et al., 2011; Stafleu et al., 2011). To test this assertion we used the full lithostratigraphic model to divide the grid and ran an IK interpolation within the individual lithostratigraphic units (Figure 11). Using the same 50% deletion test on this model, the correct answer was generated 11017 times out of 18093 (60.89%). This is only a slight improvement on the facies-based approach we advocate in this paper.

Using a facies-based approach can also highlight areas of possible error in the lithostratigraphic model, especially where units are heterolithic and it can be difficult to accurately locate lithostratigraphic boundaries (Booth and Lee, 2005). In Section 2, the *Paisley Clay Member* plots in a similar position to the highest probability of clay in the stochastic model (Figures 2 and 6). In Section 1 the lithostratigraphic model suggests that the *Paisley Clay Member* forms a continuous layer in the south eastern part of the Clyde Valley (Figure 2). However, all the simulations suggest that it may not be a continuous layer of clay (Figure 6). Such observations are crucial in understanding how groundwater and contaminants migrate through the sub-surface.

Finally, the simulations of probability for individual lithologies and the individual realisations of the SIS algorithm may be used to condition further simulations of various properties, the aim being to

produce multiple possible distributions of the property of interest. The equivalent process in the petroleum industry would be the simulation of reservoir properties such as porosity, permeability, shale volume, net-to-gross and the saturation of oil or gas within the facies framework of a hydrocarbon reservoir. Such models provide critical input to fluid-flow simulation models used to understand the performance of hydrocarbon fields (Garden et al., 2005; Sumner et al. 2005). Other stochastic modelling applications include quantifying the spatial distribution of geological risk and uncertainty in the mining industry (Benndorf and Dimitrakopoulos, 2005; Li et al., 2005), and simulating the distribution of hydraulic conductivity (Lemke et al., 2004) for a host of hydrogeological applications. Additionally, the distribution of geotechnical properties relevant to ground engineering may be studied by use of stochastic modelling; this may be particularly beneficial for the identification of problematic ground. An understanding of the lithological heterogeneity gleaned from the stochastic simulation outlined here, will allow for improved distributions of physical properties on a regional basis across the Glasgow conurbation.

7. Conclusions

In this study, our motivation has been to test whether a stochastic modelling approach could better capture the variation in lithology in highly heterolithic lithostratigraphic units than simply assuming the dominant lithology in each lithostratigraphic unit. Both stochastic methods used in the study show a slight increase in the predictive ability of the model over assuming the major component lithology. However, due to the highly clustered nature of urban datasets, the predictive ability appears to decrease with distance from the areas with a high density of control data. A more regular dataset may relieve these problems but this is rarely available in urban areas. Equally, it appears that a finer grid may more accurately be able to predict lithology at a single location, but this requires further study.

Lithostratigraphic models tend only to provide a single realisation of the geology, and it is often difficult to distinguish between those locations where the interpretation is controlled by many

observations and those where it is extrapolated. Stochastic simulation has the advantage that it produces both probabilities for each lithology and a series of plausible simulations of lithology across the study region. This can help visualise both the lithological variation and the distribution of control data. As such, it is of potentially great use to hydrogeologists attempting to understand hydraulic connectivity between units. Such probability maps and simulations are also of use to those making city-scale assessments for site investigation where large numbers (>1000) of boreholes have been drilled (e.g. large area regeneration projects) as it easily identifies areas of the model that are data poor, or very complex, that may require further investigation.

These models, however, do not give good site-specific results and will not capture stratigraphically constrained units or localised units. More detailed site-scale models could be produced for areas where large numbers of boreholes are situated. However, given the data generally available in urban environments, it is likely that there will be substantial areas with insufficient boreholes to predict lithology accurately in such heterolithic deposits.

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Table 1 Lithostratigraphic superficial units in Central Glasgow (Browne and McMillan 1989; McMillan et al., 2005). The assumed dominant lithology is highlighted in bold.

Age	Lithostratigraphic unit		Lithology	Thickness	% correct when dominant lithology is compared to lithology observed on borehole
Flandrian	Clyde Valley Formation	Law Sand and Gravel Member	Fine to coarse grained SAND with some silt and fine gravel. Bedded silt units with thin peat and organic layers.	Min = 0m Med = 0.02m Max=15.93m	3%
	Clydebank Clay Formation	Gourock Sand Member	Grey, fine to coarse SAND with some silt, clay and locally gravel	Min = 0m Med = 4.22m Max=29.97m	30%
Late Devensian	Clyde Clay Formation	Paisley Clay Member	Finely layered CLAY and some silts often orange to red-brown in colour	Min = 0m Med = 2.63m Max=36.51m	59%
		Killearn Sand and Gravel Member	Fine to medium SAND with some silt and clay layers and some gravel. Reddish-brown to orange in colour	Min = 0m Med = 0.20m Max=14.69m	60%
		Bridgeton Sand Member	Fine to medium massive SAND ; locally fine to coarse gravel and boulders occur in a sandy matrix	Min = 0m Med = 6.25m Max=35.14m	68%
	Broomhouse Sand and Gravel Formation	Ross Sand Member	Flat and ripple laminated fine-medium SAND and sandy-silt with clays and locally thin gravel layers at the base.	Min = 0m Med =2.54m Max=25.06m	6%
		Broomhouse Sand and Gravel Member	SAND AND GRAVEL deposit; mostly sand with planar and trough cross-bedsmripple and horizontal laminae, gravels typically massive or crudely bedded	Min = 0m Med = 0.03m Max=27.13m	52%
	Wilderness Till Formation		CLAY DIAMICTON , boulders, gravels and pebbles in a sandy, silty to clayey matrix.	Min = 0m Med = 5.75m Max=56.37m	62%
	Cadder Sand and Gravel Formation		Dense SAND or silty-sand with gravel and some cobbles	Min = 0m Med = 0.01m Max=20.84m	20%
	Broomhill Clay Formation		Laminated clayey SILT with sandy partings	Min = 0m Med = 0.01m Max=10.45m	Not intersected by borehole
Pre-Late Devensian	Baillieston Till	Stiff CLAY DIAMICTON , cobbles boulders, gravels and pebbles in a sandy, silty to clayey matrix.	Min = 0m Med = 0.01m Max=8.08m	Not intersected by borehole	

Table 2 Lithology dependant correlation range parameters used in the stochastic modelling. The azimuth refers to the orientation of the maximum range.

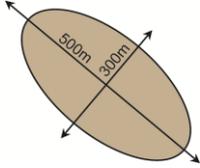
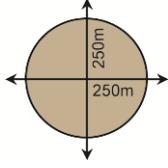
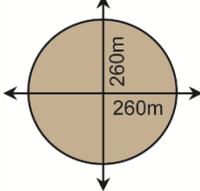
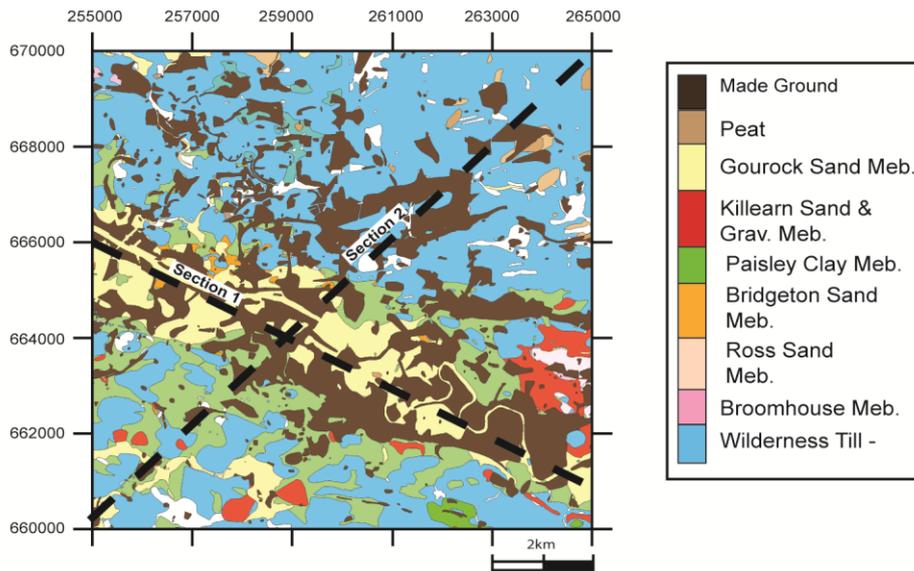
Lithology		Max Range (m)	Min Range (m)	Vertical Range (m)	Azimuth (deg)
soft clay		500	300	1	130
stiff clay diamicton		250	250	1	0
organic, silt, sand, sand and gravel		260	260	1	0

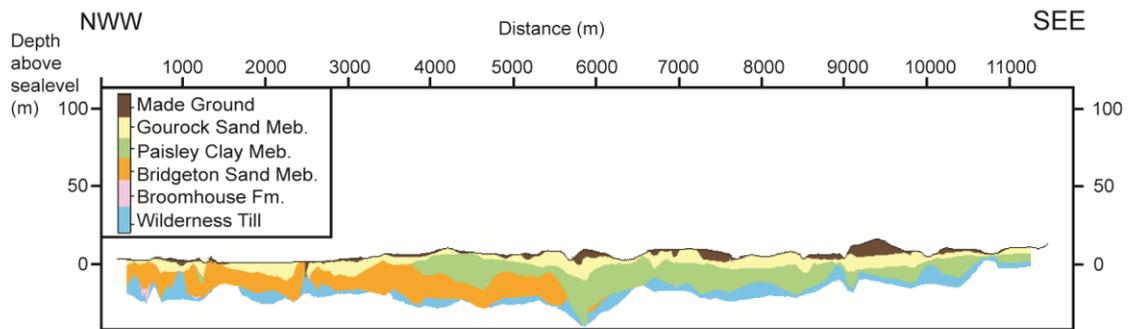


Fig. 1. Map of central Glasgow with area of this study. Grid show in British National grid (m)

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Section 1



Section 2

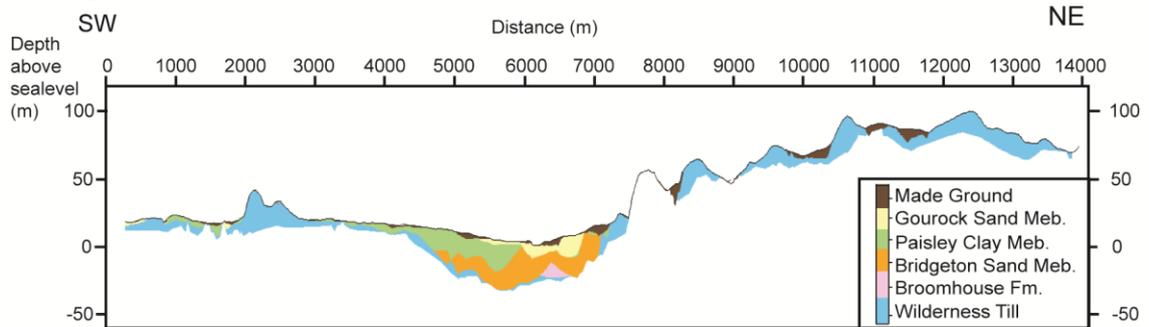


Fig. 2. Lithostratigraphic model for Glasgow (Merritt et al., 2007) showing stratigraphic relationships in Central Glasgow.

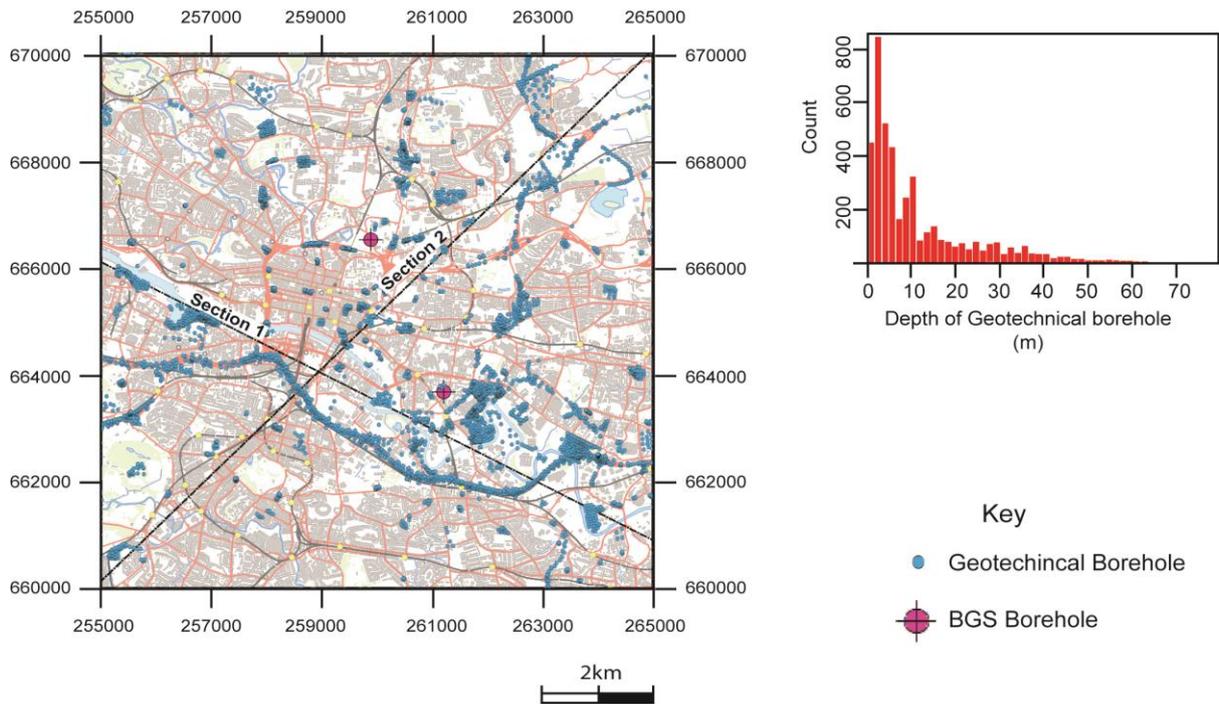


Fig. 3. Map showing the distribution of boreholes used in this study. The geotechnical boreholes were used to create the model and the BGS boreholes were used to test it. The section lines are those used to compare the deterministic and stochastic models. The histogram shows the depth distribution of the geotechnical boreholes. Contains Ordnance Survey data © Crown copyright and database right 2014.

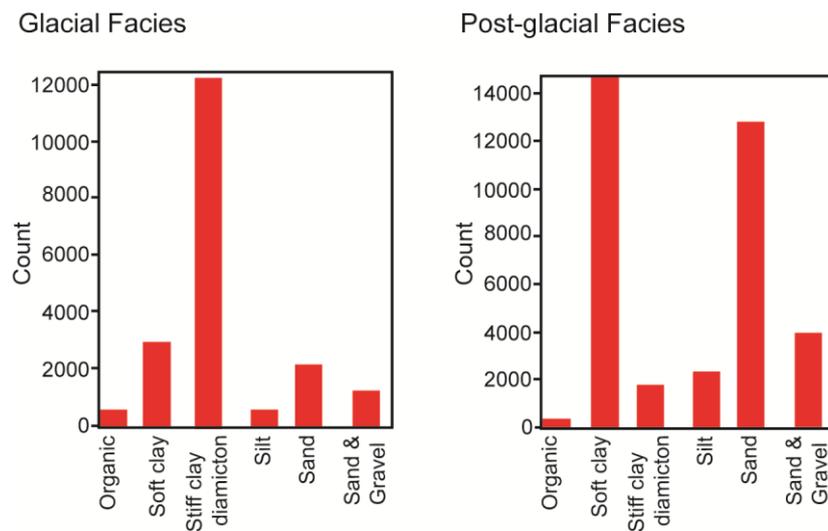


Fig. 4. Global proportions of lithologies in the two facies in the model from the borehole data.

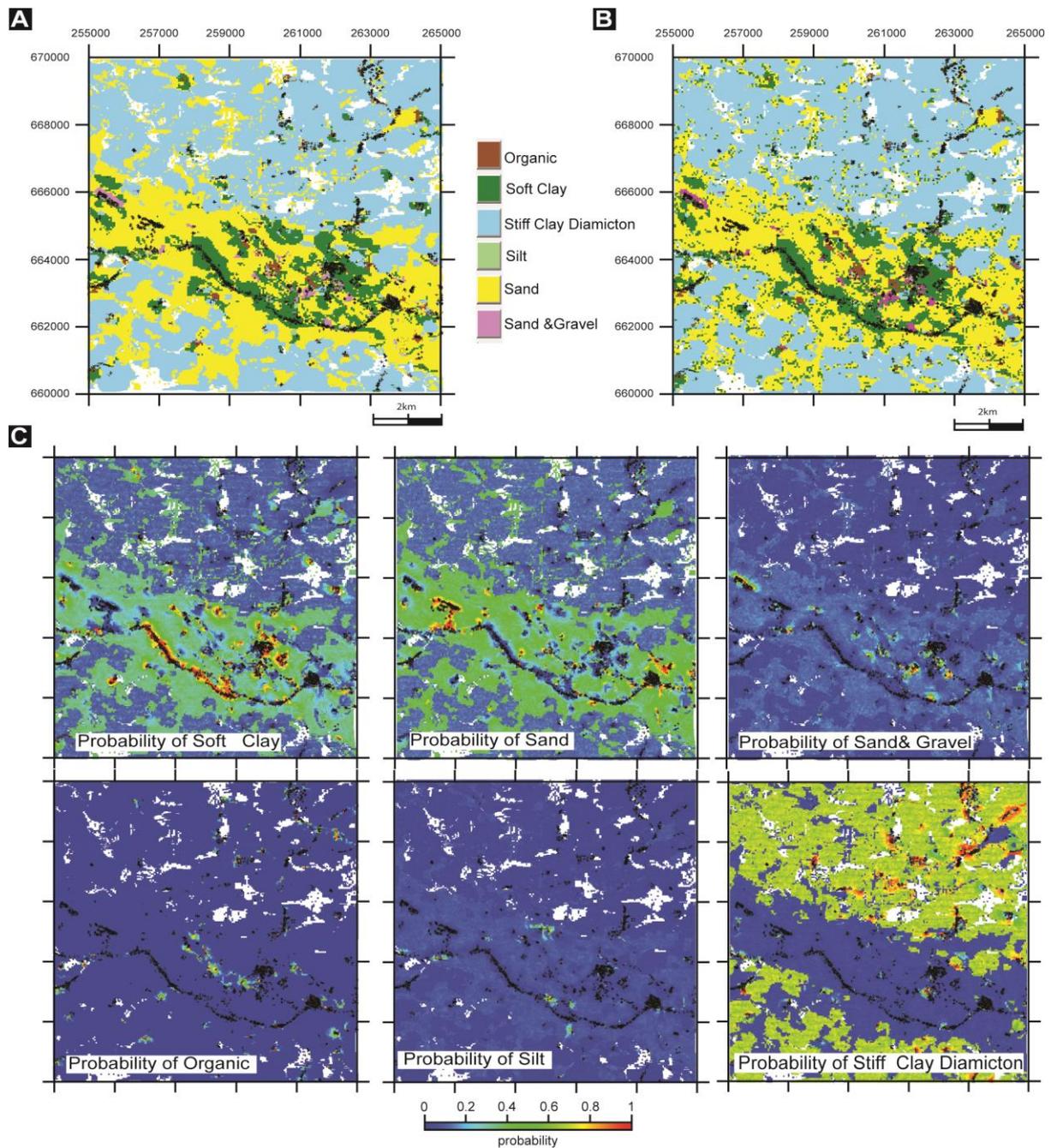


Fig. 5. Maps showing the upper surface of A) The IK model B) the SIS model most frequently occurring lithology C) the probability of the presence of separate lithologies from the SIS stochastic model. The black crosses mark the positions of the geotechnical boreholes used to create the model. The white areas are where there are superficial units and the bedrock is at surface.

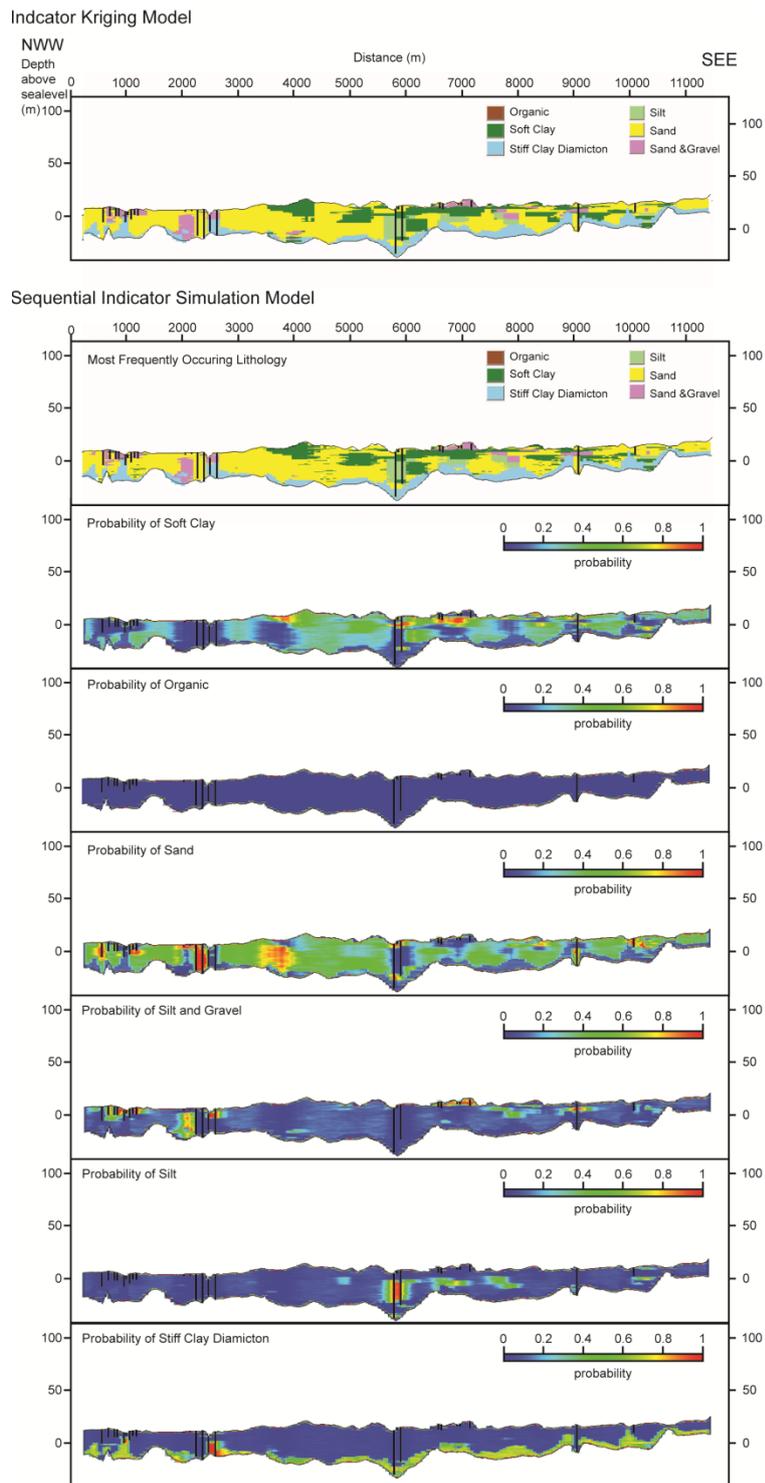


Fig. 6. Cross sections along the line of section 1 showing the IK model, the SIS model most frequently occurring lithology and the probability of the presence of separate lithologies from the stochastic model. The black lines mark the positions of the geotechnical boreholes used to create the model.

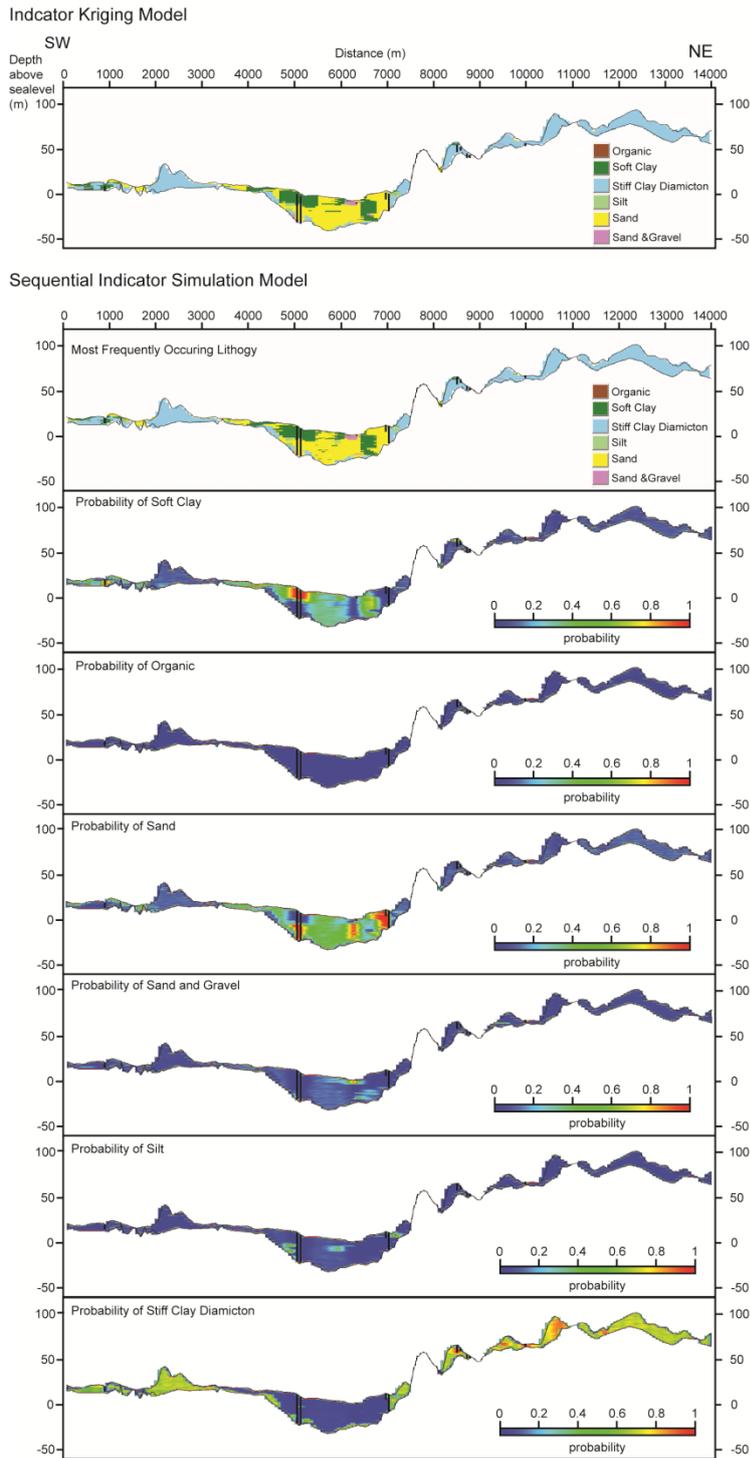


Fig. 7. Cross sections along the line of section 2 showing the IK model, the SIS model most frequently occurring lithology and the probability of the presence of separate lithologies from the stochastic model. The black lines mark the positions of the geotechnical boreholes used to create the model.

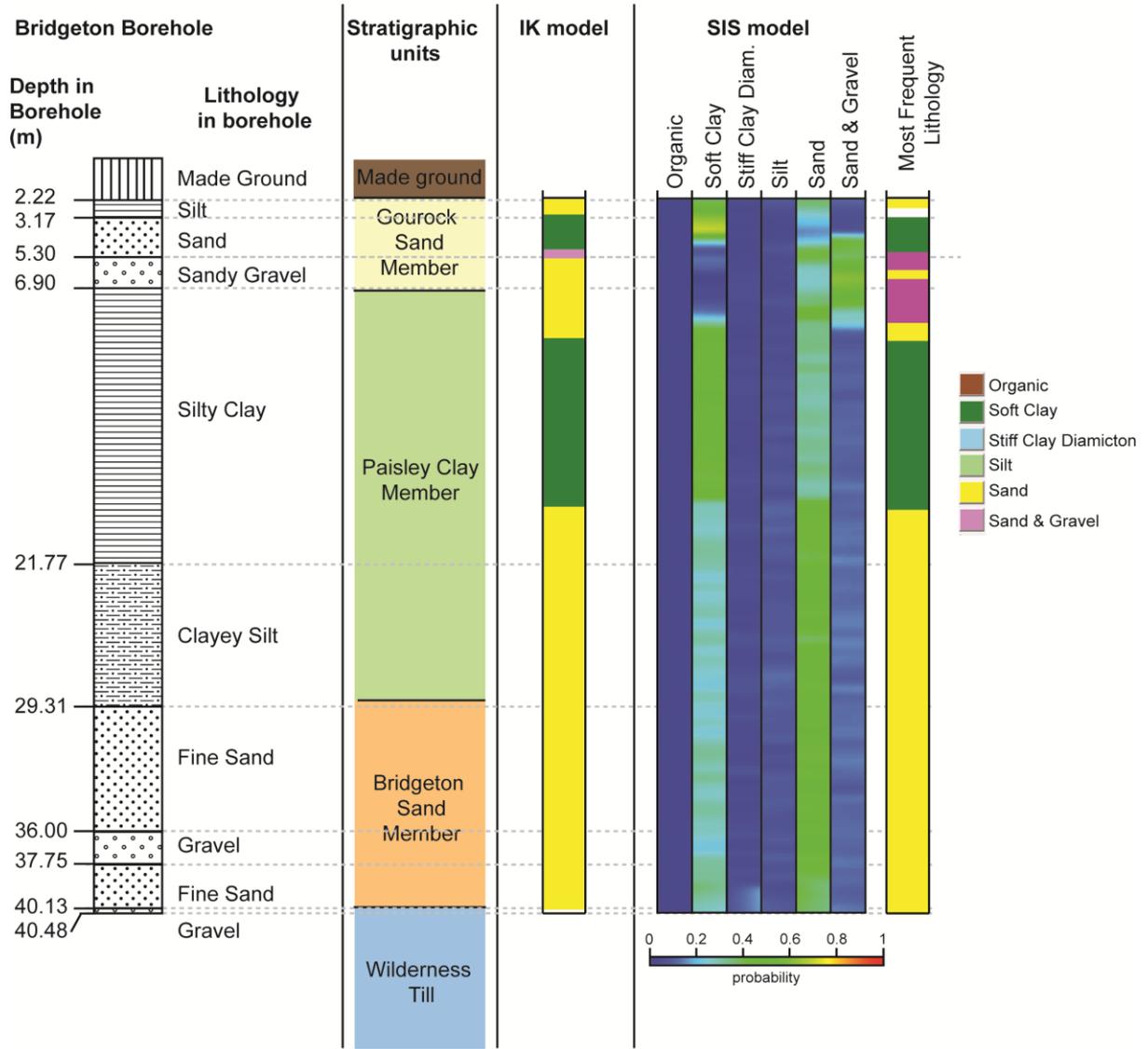


Fig. 8. Comparison of the record of what was drilled at the Bridgeton Borehole and the prediction from the stochastic models (N.B. made ground was excluded from the stochastic model).

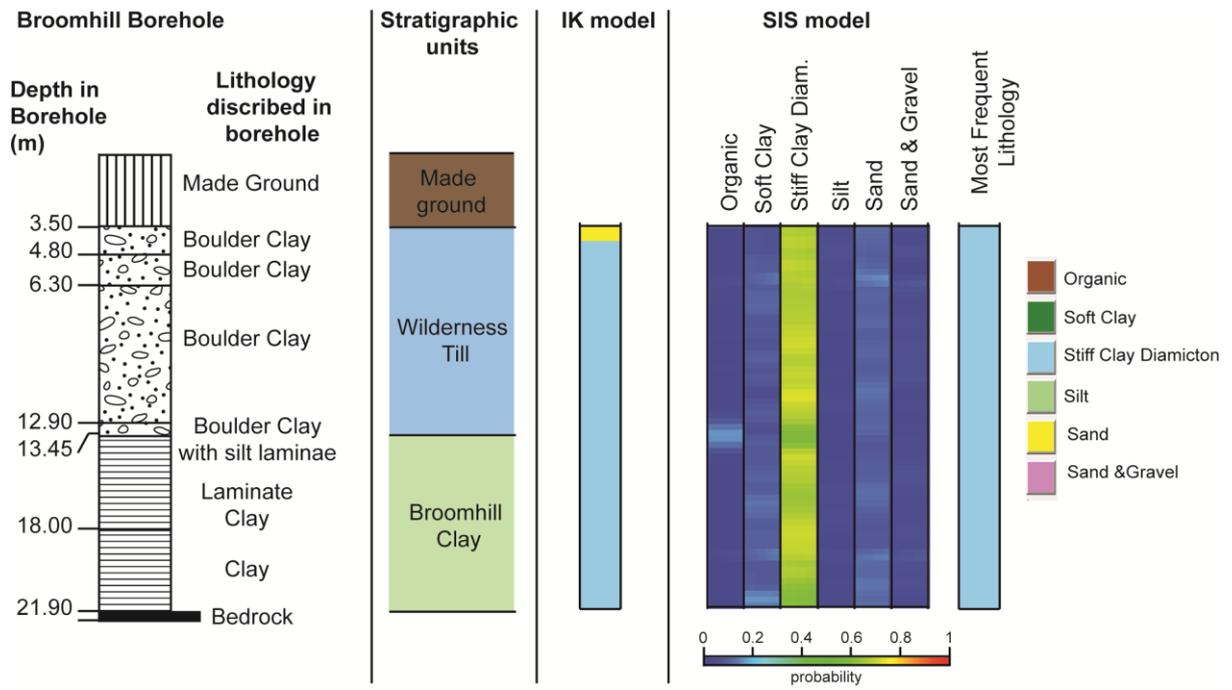


Fig. 9. Comparison of the record of what was drilled at the Broomhill Borehole and the prediction from the stochastic model (N.B. made ground was excluded from the stochastic model).

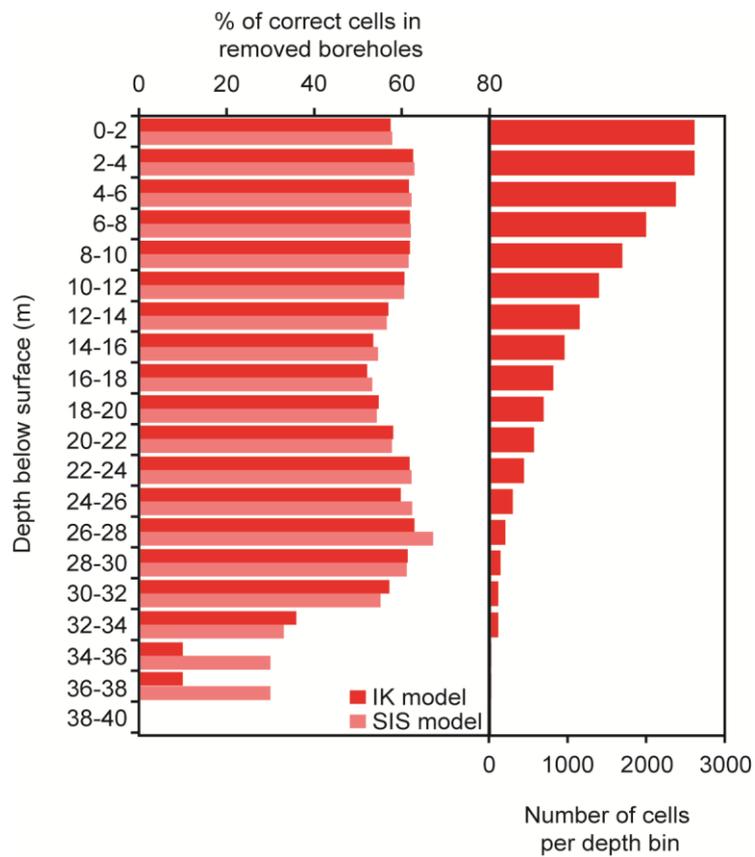


Fig. 10. The ability of the model to predict the right answer for those 50% of boreholes that were randomly deleted from the model plotted against depth from ground surface. The panel on the right shows the number of cells in the model per each depth from surface bin.

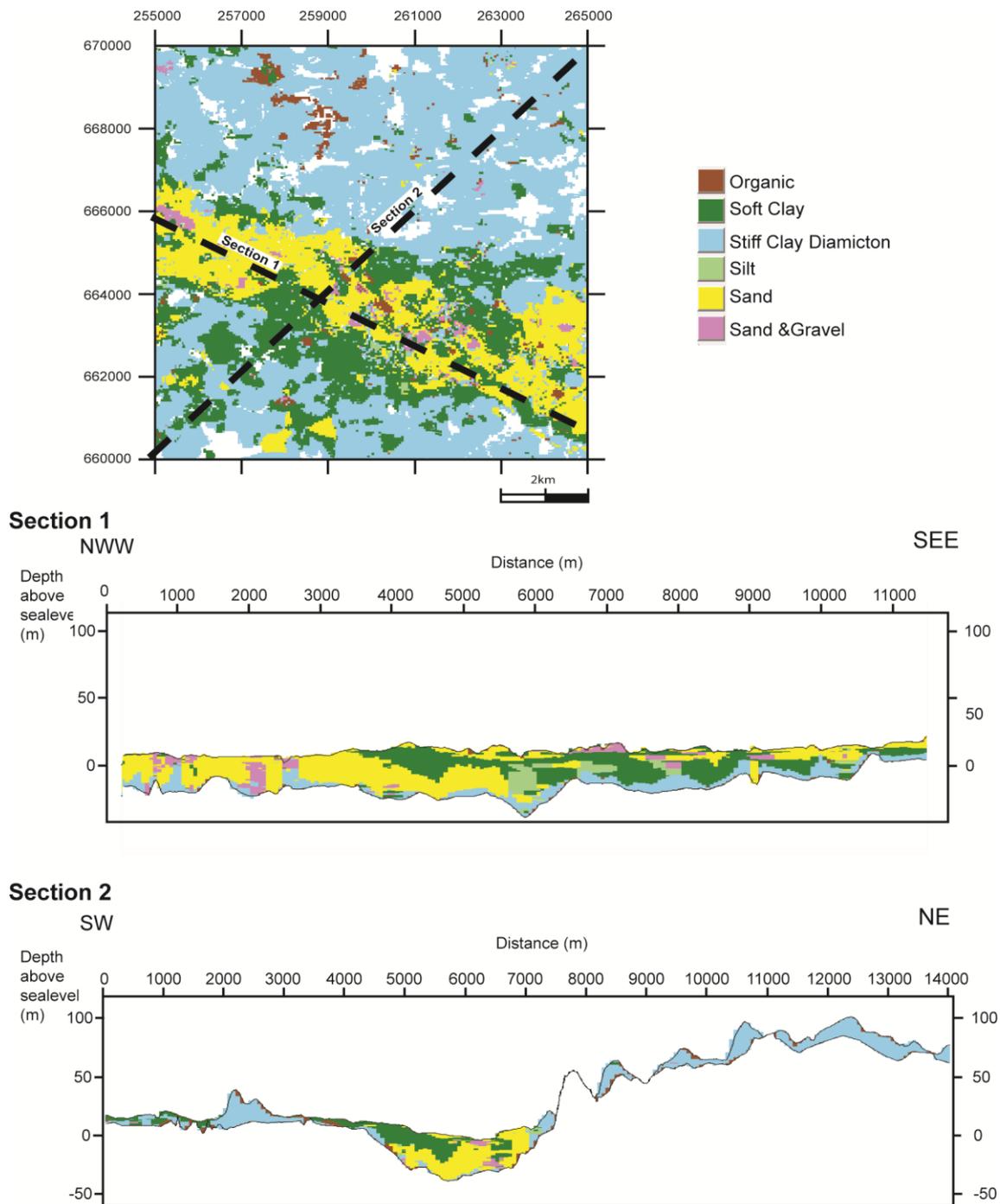


Fig. 11 A single IK realisation in a grid which has been fully divided up in to the full individual lithostratigraphic units.