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## Using numerical modelling to test the geological and groundwater conceptual understanding of a complex, layered aquifer: A case study from the Fell Sandstone, Northumbria

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**Title: Using numerical modelling to test the geological and groundwater conceptual understanding of a complex, layered aquifer: A case study from the Fell Sandstone, Northumbria.**

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**Abstract.** Groundwater abstractions from the Carboniferous Fell Sandstone, Northumbria, north-east England, provide water supply to the Berwick-upon-Tweed area. Management of these abstractions, totalling 6.5 Ml/day, by the water company along with the regulator for sustainability issues is required. Groundwater abstraction takes place from different sandstone units, which are separated by mudstones, with monitored groundwater heads showing variable responses to system stresses. To improve understanding of this complex system, various activities have been undertaken. Geological mapping and interpretation have been conducted to characterise the nature, geometry, and interconnection of the sandstone units, along with the superficial deposits. Recharge modelling has used to quantify inputs to the system and to understand the long-term water balance. A time-variant model has been implemented to simulate groundwater flow in the sandstone units and to quantify the groundwater balance. The work confirms that the Fell can be split into seven discrete sandstone units, separated by low permeability mudstones, but they are not necessarily laterally connected. There is a range of timescales of groundwater response to recharge events from slow (six months) to very rapid (~1 day). These findings confirm the complexity of this groundwater system and offer lessons for similar sandstone systems in the UK and worldwide.

## **1 Introduction**

Sandstone aquifers form globally important groundwater systems. Their relatively high porosity, and therefore storage, provides useable groundwater resources in many parts of the world. Examples include the Nubian sandstone aquifer in north Africa (MacDonald et al., 2012), the Great Artesian Basin in Australia (Hayes et al., 2019), the Guarani of South America (Hirata & Foster, 2020), and parts of the US (e.g. High Plains Aquifer; (Korus Jesse et al., 2022) ). In the UK, Permo-Triassic sandstone aquifers are of significant importance for water supply purposes, providing the second most exploited groundwater resource after the Cretaceous Chalk aquifer. Whilst Permo-Triassic sandstones are the most widely studied – e.g. (Colyer et al., 2021; Lafare et al., 2021), with both Permian age (MacDonald et al., 2003) and Triassic-age sandstones (Medici et al., 2019) receiving attention – other, minor sandstone aquifers also contain important water resources for local communities. One such

example is the Carboniferous age Fell Sandstone located in north east England, which has provided important water supply for the Berwick-upon-Tweed area since the early 1900's (Hodgson et al., 1971), as well as being exploited for geothermal purposes under Newcastle-upon-Tyne (Younger et al., 2016). Belying its relatively small outcrop area, it is geologically and hydrogeologically complex (Turner et al., 1992) and has not had the commensurate attention that other sandstone systems have received to understand it fully.

This paper provides a summary of the geological and modelling activities conducted to develop an updated conceptual groundwater flow model of the Fell Sandstone in the Berwick-on-Tweed area. We also present the first attempt of applying distributed numerical modelling to simulate groundwater dynamics of the Fell sandstone, a complex layered aquifer, which has been used to test the updated conceptualisation, and to assess the sustainability of the abstractions. The main findings resulting from these recent studies demonstrate the complexity of this groundwater system and offer lessons for similar layered sandstones both in the UK and worldwide.

### *1.1 Summary of previous investigations of the Fell Sandstone in Northumberland*

The first geological assessments of the Fell Sandstone were published in the middle of the twentieth century by Robson (1956) and Smith (1967) focussing on the sedimentological nature. However, the earliest comprehensive hydrogeological study was provided by Hodgson et al. (1971). They examined meteorological, hydrogeological and geochemical data to develop a conceptual understanding of groundwater flow in the Fell Sandstone in the Berwick area, including Berwick itself, which has been subject to groundwater abstraction (Figure 1) since the late 1930s. A recharge value of 392 mm/a was estimated for the whole Fell Sandstone outcrop, and it was concluded that the overall water balance was showing a surplus. Hodgson et al. (1971) also report results of pumping tests in two abstractions boreholes ("Thornton" and "Borehole A") showing transmissivities in the order of 50 m<sup>2</sup>/d. Groundwater flow direction was assumed generally towards Berwick to the north-east, while chemical analysis of groundwaters samples indicated mainly neutral pH and chemically moderately hard waters with limited evidence of saline intrusion in Berwick. An area of reduction in the main chemical determinants (e.g. TDS) was observed around Borehole A thought to be related to pumping and induced recharge (Hodgson et al., 1971). Based on the results of these investigations, Hodgson et al. (1971) concluded that there was potential for further exploitation of the Fell Sandstone and in particular, the suitability for the provision of a groundwater supply for the Berwick area.

Turner et al. (1992) then built on previous geological and hydrogeological studies to provide conceptualisation of the aquifer system consisting of a sequence of seven distinct sandstone

units separated by mudstone units. From the top to the bottom of the stratigraphic sequence, the sandstone units were named “South Ord”, “Murton Craggs”, “Murton Deane”, “Peel Knowe”, “Middle Ord”, “Royalty” and “Thornton Park”. This conceptualisation has been the mainstay of any hydrogeological investigations since.

There is some evidence suggesting karst behaviour in the Fell Sandstone, which was first identified and reported by Mullan (1989). Some indications of karst behaviour in boreholes as a result of fracturing and removal of weakly cemented sandstone are also reported in the BGS/EA Minor Aquifer Properties Manual (Jones et al., 2000). The theme of karstification was further developed by Self et al. (2005), who made the case for cave development and provide proof of the existence of sinking streams.

Over recent decades there has been a significant amount of work undertaken by environmental consultants on the conceptualisation of the aquifer system. Two main studies, commissioned by the Environment Agency (EA) and undertaken by Entec (now WSP, previously Wood and AMEC), presented a conceptual model of groundwater flow in the Fell Sandstone (Entec, 2009) and a revised recharge model and water budget using new data (AMEC, 2012). These studies were incorporated into one undertaken by Northumbrian Water Limited (NWL) as part of the National Environmental Programme (NEP) work. This study (NWL, 2018) builds on the AMEC work along with an MSc thesis completed at Imperial College, London (Colyer, 2018) and provides a more refined geological and hydrogeological understanding of the area. In terms of hydrochemistry, the studies of (Entec, 2009), (NWL, 2018), (Dearlove & Schwartz, 2022) and the more detailed EA nitrate report (2016) presented a more detailed discussion of the background groundwater geochemistry as well as the nitrate pollution in the aquifer.

Before this study, there have been few applications of groundwater modelling to study the Fell Sandstone aquifer. However, these only focussed on the estimation of the water balance without considering distributed models of groundwater flow dynamics. Examples of these previous modelling applications include a systems dynamic approach (Markou, 2013) and a lumped parameter model (Colyer (2018) based on AquiMOD (Mackay et al., 2014). The latter showed that the Fell Sandstone response to recharge has significant spatial variability.

## 2 Study area description

### 2.1 Location

The Fell Sandstone is situated in Northumberland, north east England, with Berwick-upon-Tweed to the north-east (Figure 1). The outcrop describes a thin curve adjacent to the Cheviot Hills with topography rising from sea level to a maximum of 440 m above Ordnance Datum (a OD). The outcrop forms a craggy escarpment with dip slopes to the south-east leading down to the River Tweed and eventually the North Sea. The land use is predominantly arable except the urban centre of Berwick. Long-term average annual rainfall for the period January 1987 to December 2018 is 695 mm/a, with variability in precipitation controlled by the topography. The main river in the area is the River Tweed, which is fed by a number of small tributaries running off the outcropping areas of the Fell Sandstone.

### 2.2 Geology

The region's bedrock succession and glacially dominated superficial geology is depicted in 1:50 000 scale map data (BGS, 1977) and summarised by Stone et al. (2010). The Carboniferous-age Fell Sandstone Formation has been the subject of extensive sedimentological studies (Smith, 1967; Turner et al., 1987; Turner et al., 1992; Turner et al., 1993). Ford et al. (2019) provide a re-interpretation of the geology of the study area based on remote sensing, field-based studies, and borehole correlation (Figure 2a). The following geological summary and cross-sections (Figure 2b) are based on Ford et al. (2019).

In the Berwick-upon-Tweed area, the 225 to 350 m thick Fell Sandstone mostly comprises interbedded sandstone, siltstone and mudstone. Seven main sandstone units and several lesser sandstone-dominated layers are recognised. Sandstone units vary in thickness (up to 20 m) and lateral extent. The sandstone units are commonly medium- to coarse-grained, moderately rounded, moderately sorted and ubiquitously cross-bedded. Mudstone units observed in drill core (e.g. Murton Craggy Bogs Observation borehole 1) are dark reddish brown, and lack internal structure (Dearlove et al., 2022).

The Fell Sandstone is underlain by the Ballagan Formation, a succession of thin and thick sandstones, mudstones and siltstones, with 'cementstones'. Due to lithological similarities between the formations (as reported in borehole records) and a lack of outcrops in the study area, the base of the Fell Sandstone is poorly constrained in the geological cross-sections.

The Fell Sandstone is overlain by the Scremerston Formation, comprising alternations of sandstone, siltstone, mudstone and coal, with occasional dolomite or limestone beds.

Descriptions of the Fell Sandstone that are based on its full geographic extent (BGS Lexicon) cite limestone, coal and seatearth (deposits underlying coal seams) as 'subsidiary' or 'trace lithologies'. However, a detailed review and correlation of borehole records indicates that these lithologies are absent from the formation in the study area. Hence, for this work the base of the Scremerston is taken below the lowest recorded interval of limestone, coal (or associated seatearth, fireclay etc.).

In the study area to the south of Berwick-upon-Tweed, the Fell Sandstone generally dips towards the southeast by 8° to 12°. An asymmetrical southeast-plunging anticline in the Berwick-upon-Tweed area is associated with dips of up to 25°. Two mapped faults exist in the study area to the north and south of the Bleak Ridge borehole, cutting west–east. These structures are inferred to be normal and have downthrows of up to 40 m to the north. Current structural mapping in the study area underrepresents the extent of faulting and associated deformation. It is highly likely that unmapped faults are present, and that these may limit the lateral continuity of the sandstone units or juxtapose stratigraphically different units.

The superficial geology of the study area (Figure 3) broadly consists of: glacial till (semi-continuous sheets in low-lying parts of the study area and irregular patches on the east-facing slopes); patches of sand and gravel (associated with the till areas); head (ribbons between till deposits and areas of no superficial cover, especially in the south of the study area); river alluvium and accumulations of peat (occupying modern-day drainage system and topographic depressions, including the Thornton Bog area).

### 2.3 Hydrogeology

The main groundwater system consists of sandstone bodies within the Fell Sandstone, which form different aquifer units separated by less permeable mudstone units. Flow in the sandstone is assumed to be predominantly intergranular, but there is some evidence of fractures in the core as well as karstic features, which have been identified further south towards Wooler, i.e., Routin Lynn Cave (Mullan, 1989).

Relatively few pumping tests have been undertaken in this area, e.g. see Jones et al. (2000). These indicate a relatively low transmissivity (T) with values in the order 100 m<sup>2</sup>/d, a storage coefficient (S) of about 1×10<sup>-4</sup>, and a specific yield of about 10%. Entec (2009) report transmissivities estimated from pumping tests in three different boreholes ranging between of 52 and 126 m<sup>2</sup>/d (min to max). NWL (2018) report values of 50–100 m<sup>2</sup>/d for the Borehole E borehole 100 m<sup>2</sup>/d for the Borehole A borehole, 100 m<sup>2</sup>/d for Borehole C and D, 50–70 m<sup>2</sup>/d for the Borehole F; and 125 m<sup>2</sup>/d Shoreswood Farm borehole

Ambient regional groundwater flow direction is difficult to discern from analysis and interpolation groundwater heads measured in boreholes given the relatively sparse monitoring network and the influence of abstractions. Historic analysis presented in Hodgson et al. (1971) seems to suggest the groundwater flow direction is north/north-east towards Berwick. However, this simplistic interpretation is unlikely to represent the current state of the flow field, given the layered nature of the aquifer and the cones of depression caused by the abstractions.

A conceptual groundwater balance capturing the main components can be defined as follows (e.g. (Fetter, 2018)):

$$\text{recharge} + \text{SW inflow} + \text{GW inflow} = \text{abstraction} + \text{springflow} + \text{GW outflow} \pm \text{change in storage}$$

The main inflow is likely to be rainfall recharge, predominantly direct, i.e., occurring where precipitation directly infiltrates at outcrop. Secondary to this is the runoff from other adjacent areas (SW inflow) and any exchange with other groundwater units. The main outflow is likely to be NWL abstraction and other local abstractions with secondary outflows being springflow and limited baseflow to streams.

Infrequent spot gauging is carried out at the streams draining the area, namely Hornclyffemill Burn and Newbiggin Dean. It has been reported that groundwater levels are below the base of the stream bed and the streams could be losing flow to the sandstone units (Environment Agency (2016)).

The main features of the conceptual model are how “layered” the system is thought to be with sandstone units separated by mudstone. The main inflows are rainfall recharge and subsurface runoff from the mudstone. Groundwater flow is along the sandstone units, dipping down towards the centre of the basin. Faulting may play a part in restricting flow within the aquifer.

#### 2.4 Geochemistry

Groundwaters are typically Ca-Mg-HCO<sub>3</sub> type, with some exceptions including higher chloride, sulphate and sodium-potassium water in localized areas. The piper diagrams presented in Entec (2009) show relatively uniform chemical compositions of the borehole waters, while those presented by NWL (2018) seem to indicate a wider heterogeneity.

In terms of impact of anthropogenic activity on groundwater quality, nitrate pollution is an issue in the catchment (Dearlove et al. (2022)). Elevated concentrations of chloride are also observed in boreholes mainly in the urban area of Berwick, but values are very much lower

than sea water concentrations and have been interpreted as not likely related to saline intrusion (Entec, 2009). The Environment Agency (2016) examined land use (soil sampling for soil mineral nitrogen) and measured nitrate concentrations in a number of boreholes in the area. In general, nitrate concentrations are increasing; in particular, Thornton Farm and Royalty boreholes which showed concentrations above the drinking water standard (DWS) and upwards trends. Upward trending concentrations were also observed in other boreholes (Boreholes B, C, D and E) albeit with nitrate concentrations below the DWS. Other boreholes showed an downwards trend, notably Shorewood Loan and Peel Knowe. Rates of movement of nitrate through the unsaturated zone were estimated to be in the order of 3 m/a in the unsaturated zone and travel times from the water table to abstraction boreholes between 5.3 and 13.4 years in the saturated zone (Environment Agency, 2016).

### **3 Methods and materials**

The following section describes the activities conducted to revise the geological understanding, to quantify aquifer recharge and estimate the water balance, and to implement a numerical groundwater flow model of Fell Sandstone in the area immediately west of Berwick.

#### *3.1 Revision of the geological understanding*

The first step in the revision of the geological understanding was to identify relevant data sources and collate them into a systematic dataset (see Table 1). An initial set of over 350 boreholes was identified and then a sub-set identified having depth greater than 10 m. These >10 m deep boreholes were coded by an agreed internal BGS protocol. Coding of the boreholes recorded as much sedimentological information (grainsize, composition texture, structure etc.) as possible to aid subsequent correlation. Of the initial borehole records identified, 83 have been used in the construction of the schematic cross-sections and revised 1:50,000-scale geological linework. The understanding of the 3D geology was supplemented with the examination of cores where available as well as fieldwork involving visits to quarries and other surface outcrops. A number of field sedimentary logs were recorded at the available outcrops in the region (Murton High Crag and two localities in Shoreswood; Quarry and field cutting). These sedimentary logs were taken to identify the sedimentological architecture of the exposed sandstones. Building on the 83 coded boreholes as well as other information, schematic cross-sections were created using BGS



in-house software 'Groundhog'<sup>1</sup> using a Bald Earth digital elevation model (DEM) as the capping surface.

### 3.2 Recharge modelling and water balance

Recharge was estimated with the distributed recharge model ZOODRM (Mansour et al., 2018). ZOODRM uses the UN Food and Agriculture Organisation (FAO) method (Allen et al., 1998) to estimate evapotranspiration and excess soil water, and the excess water is split into surface runoff and recharge according to run-off coefficients. Surface runoff is routed across the land surface and can re-infiltrate into non-saturated soil: for example, in this case, runoff generated on the mudstone may infiltrate into downslope sandstone outcrops.

The datasets used in the recharge modelling are shown in Table 2. The BGS Parent Materials dataset (Lawley, 2014) was used to define soil type, although modifications were made to ensure consistency with sandstone outcrop mapping (Figure 4). The soil types were translated into soil properties (wilting point and field capacity) with the Hydrology of Soil Types (HOST) classification and BFIHOST used to define runoff coefficients (Boorman et al., 1995). Drainage channels were incorporated into the model in the area of peat soil (Figure 4) according to Ordnance Survey mapping.

The extent of the recharge model is shown in Figure 4 which is greater than the MODFLOW groundwater flow to take into account surface water catchments. The model was gridded at 25 m resolution in order to capture the spatial variability of the geological outcrop, to enable runoff recharge to be represented, and to ensure compatibility with the groundwater flow model (see below). The recharge model extends to the fault in the south and to the mouth of the River Tweed in the north. No continuous streamflow gauging was carried out within the recharge model area; however, infrequent (less than monthly) spot gaugings were obtained from the EA for two streams flowing off the Fell Sandstone (Figure 4) for the period 2012–2018. The model was run from 1987 to 2018 to counter climatic variation. Recharge from the first year of the model run, 1987, wasn't used to avoid any inaccuracies of calculating recharge with the initialization of soil moisture at zero..

Previous 1D groundwater modelling (Colyer, 2018) – as well as visual inspection of the groundwater hydrographs – suggested a strongly damped seasonal signal in recharge across much of the Fell Sandstone. Recharge was, therefore, smoothed before being

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<sup>1</sup><https://www.bgs.ac.uk/research/environmentalModelling/groundhogDesktop.html>.

incorporated into the groundwater model. The recharge was averaged over 6-month periods (January to June and July to December).

### 3.3 Groundwater flow model

A 3D numerical model has been implemented using the finite-difference code MODFLOW 2005 (Harbaugh, 2005) to simulate time variant groundwater flow in the Fell Sandstone aquifer system. A finite-difference model code was chosen as it allowed a flow balance at each node alongside reasonable runtime. MODFLOW allows solution of the partial differential equation describing groundwater flow in porous or equivalent porous media given a set of input hydrogeological parameters, boundary and initial conditions, and the parameters defining sink/source terms such as groundwater abstractions and aquifer recharge rates. The purpose of the implemented model was to simulate the overall groundwater dynamics in the study area (Figure 1), with particular emphasis on the understanding and quantification of groundwater fluxes within and between the different sandstone units under realistic abstraction scenarios

The MODFLOW-2005 numerical model was implemented in two stages: a preliminary model based on previous geological understanding was initially implemented to test the interaction of the main sandstone units (Bianchi et al., 2019). This was followed by a revised second model (Bianchi et al., 2020), which took into account the novel geological understanding (Ford et al., 2019) and considered an expanded modelling domain to the south-west including the area surrounding the NWL Borehole F (Figures 1 and 5).

The model domain was discretised with a block-centred finite difference grid consisting of square cells with sides equal to 25 m, organised in 156 rows and 336 columns. In the vertical direction, the domain was discretised into seven layers each representing a single sandstone unit. The correspondence between model layers and current geological interpretation and historical nomenclature of the sandstone units is as follows:

- Layer 1: "South Ord"
- Layer 2: "Murton Crags"
- Layer 3: "Murton Dean"
- Layer 4: "Peel Knowe"
- Layer 5: "Middle Ord"
- Layer 6: "Royalty"
- Layer 7: "Thornton Park"

The mudstone units separating the sandstone units (Figure 5) were simulated as "quasi 3D confining beds". With this choice, groundwater flow is not explicitly simulated, but their

thicknesses and hydraulic properties control the rate of vertical flows between two overlapping sandstone units. In the model, the thicknesses of both the sandstone and mudstone units vary in space. For both the sandstone and the mudstone layers, the thickness values assigned to the corresponding cells of the numerical grid were estimated from interpolation of values picked at borehole locations in eight cross-sections, which were interpreted as part of the revision of the geological understanding of the study area (Ford et al. (2019)). Inactive cells, that is cells that are not considered in the numerical solution of the groundwater flow equation, were also used to map the geometry of the different sandstone units in the model. In particular, for each unit, the cells of the corresponding layer located to the north-east of the outcropping areas (Figure 5) were considered as inactive. Moreover, for layers 4 and 6 (corresponding to “Murton Dean” and “Royalty” units, respectively), inactive cells were also assigned to areas of the modelled domain where the geological interpretation indicated that lateral continuity of the sandstone units is interrupted.

Recharge rates applied to cells representing the outcropping areas of the different sandstones units (Figure 1) correspond to the output of the ZOODRM recharge model. Given the model area did not extend to the River Tweed meant that this was not included as a boundary condition. Instead, general head boundary conditions (GHB) were assigned to each layer along south-west and north-east boundaries of the domain to allow groundwater inflows or outflows across these boundaries. The boundaries also considered the regional groundwater flow, assumed from the area to the south-west of the modelled domain to north-east towards Berwick-upon-Tweed and the coast. Given the lack of specific data, the magnitudes of these fluxes were estimated during the model calibration by adjusting the conductance and reference head values of the GHB cells.

Time variant groundwater flow was simulated using daily time steps and monthly stress periods (372 in total) from the 1/1/1988 to 1/12/ 2018. During the simulation, net recharge and groundwater abstraction rates were updated at every stress period. Groundwater abstractions from the six NWL pumping boreholes (Boreholes A-F) were simulated with the MODFLOW Well Package, considering monthly averages of the daily abstraction rates provided by NWL. The location of the abstraction cell within a particular model layer and sandstone unit was chosen after integration of borehole construction data into the geological cross-sections. The initial condition for the transient flow simulation was the groundwater head distribution at the end of a steady-state run considering average recharge and abstraction rates.

Model calibration was performed with a trial-and-error approach in which input model parameters were varied until a satisfactory match was found between simulated and

measured hydraulic heads in 18 boreholes. The parameters considered for calibration include uniform values for the horizontal and vertical hydraulic conductivity (K) and storage coefficient of the sandstone units, uniform vertical hydraulic conductivity values for the mudstone units, the conductance and head values of the GHB boundaries for the different layers, and the exponents in the exponential equations describing the vertical reduction of K and S with depth. The later was used to represent vertical variation in hydraulic parameters within a single layer of a groundwater model, e.g. (Rushton et al., 1989).

## 4 Results and discussion

### 4.1 Geological understanding

Collectively, the units within the Fell Sandstone were deposited within a fluvial-deltaic setting, with the sandstone units representing the higher energy deposits (compared to the mudstone) generated within the river channels and on the delta that these channels feed into. The mudstones within the Fell Sandstone are either the product of floodplain deposition (associated with the channel sandstones) or were laid-down within shallow marine environments. However, it was not possible to discriminate between these two types of mudstone, though the ability to do so could allow for more accurate subdivision and correlation of the Fell Sandstone.

Limited surface outcrop examples in the region show that the sandstones are commonly medium to coarse grained, moderately rounded, moderately sorted and ubiquitously crossbedded. Crossbedding in the sandstones was created primarily by the downstream migration of various sized subaqueous sand dunes. These sand dunes migrated down river (in the palaeo-drainage direction) and, as a result of the rate of sediment supply within the system, were able to be preserved as stacked successions of crossbedded lithofacies. The size of the crossbedding sets is controlled primarily by the maximum depth of water in which the sand dunes were deposited. Generally thicker sand bodies (e.g. Murton Craggs and Peel Knowe equivalents) are more likely to contain well-developed and thicker crossbedded units. Large-scale crossbeds (>2 m thick, for instance) could be used to inform the identification and correlation of thicker sand units or, possibly, to distinguish thinner sand units in which well-developed and thicker crossbedding may be less likely (e.g. South Ord, Thornton Park equivalents).

At a larger scale, the separation of the succession into predominately mudstone- and sandstone-dominated layers (e.g. Table 3) is likely driven by cyclical changes in the sea level during the period of deposition of the Fell Sandstone (e.g. Turner et al. (1997)). The

start of the deposition of the sandstones (their bases) likely represents periods of relatively low sea level, whereby the rivers of the Fell Sandstone flowed out over the continental shelf for greater distances to reach the ocean into which they drained. The fall in relative sea level would have also had the effect of causing the fluvial system to incise and erode underlying material. Some of the mudstones including the laterally more persistent interleaving mudstones between the sandstones (Table 3) are likely to be of marine origin and record periods of higher sea levels, whereby sea water would have inundated areas previously occupied by the fluvio-deltaic systems. Repetitions and cycles of sea level rise and fall are ultimately responsible for the gross-scale geometry of the succession.

Examining the Murton High Crag and Shoreswood Quarry sedimentary logs (Figure 6) show a remarkably similar succession and lithofacies ordering. The similarities provide a point of evidence to these two outcrops belonging to the same named sandstone equivalent. The thicker succession at Murton High Crag and the inclusion of small pebbles in the 'trough crossbedded coset' lithofacies (c.f. the Shoreswood Quarry log) is interpreted as reflecting more central and marginal channel locations respectively. A central channel location is likely to contain deeper and faster flowing water allowing the lithofacies to be thicker and contain higher energy deposits (e.g. including pebbles). Channel marginal settings are generally located in shallower and quieter water, though still subject to the same general conditions as the related central channel position.

The presence of a laterally extensive (>40 m), highly deformed horizon of crossbedded sandstones at Murton High Crag is interpreted as a 'seismitite'. Seismitites are 'normal' deposits which have deformed by local- to regional-scale tectonic event(s) that cause 'slumping' in the non-lithified (loose sediment) deposits. If these facies are seismitites, the tectonism occurred during the deposition of the Murton Crag Sandstone and was geologically instantaneous, as the underlying and overlying lithofacies are not deformed.

The mudstone units have not been observed in outcrop but have been identified in borehole logs and the core taken from the Murton Craggy Bogs Observation borehole 1. This revealed that much of the mudstone represents stacked palaeosols (fossilized Carboniferous soil profiles). These are dark reddish-brown mudstones with no evidence of internal lamination and often exhibiting yellow mottles and faint bluish grey streaks. The reddening indicates the palaeosols were not waterlogged when formed, but were in oxidising conditions where iron minerals formed  $\text{Fe}^{3+}$ . These mudstones were originally deposited as siltstones in fluvial overbank floods (floodplain deposits) on the Carboniferous river floodplain. Subsequent and repeated colonization by plants and the formation of palaeosols altered the silt to mud.

As previously mentioned, some of the mudstone units were formed in a marine environment. The interval between 38–44 m in the Murton Craggy Bogs Observation Borehole 1 contains units with climbing or symmetrical ripples and intense bioturbation (trace fossils resulting from the action of plants and animals). In-situ bio-activity in an “optimum” environment for life to survive – deposition below water, in an oxygen-rich water column, is likely within the photic zone. Unlike the palaeosols, these units were probably deposited in a large standing body of water, such as a lake or lagoon. The level of bioturbation suggests that this was most likely to have a marine connection. The interbedding and overprinting of the bioturbated intervals and the palaeosol suggests that, in this interval, the rocks were deposited at the very edge of a water body.

Existing 1:50,000-scale geological maps show considerable faulting to the east of the study area within the Scremerston Formation and succeeding parts of the Yoredale Group. Mapped faults are generally oriented west-east to northwest-southeast and exhibit throws of several tens of metres. Only two faults have been identified by mapping to affect the Fell Sandstone or the Ballagan Formation within the study area (Figure 2a). This apparent difference in fault density may be due to the relative lack of observable evidence to support faulting in the Fell Sandstone and Ballagan Formation when compared to the overlying succession including the coal-bearing Scremerston Formation. It is assumed that mine plan data and more detailed mapping have resulted in a greater number of faults being recognised.

The revised interpretation shows two faults in the south of the study area (Figure 2a): west-east trending Shoreswood Fault is inferred to have a downthrow to the north of approximately 40 m and the east-southeast trending Bleak Ridge Fault is inferred to have a downthrow to the north of up to approximately 20 m on the eastern side of the Fell Sandstone outcrop. They have been inferred from recent geological mapping, the geometric reconstruction of the succession based on borehole data and topographic evidence. In both

cases, the faults have been informed by existing geological interpretations and this work has extended to join previously mapped structures in the Scremerston Formation.

#### 4.2 *Net recharge and water balance*

Long-term average distributed recharge generated by ZOODRM can be seen in Figure 7. Recharge on the outcrop varies between 150 and 225 mm/a. This range is somewhat lower than previous assessments (e.g. Infiltration of 392 mm/a in Hodgson et al. 1971). Estimated values for the components of the water balance extracted from the recharge model are presented in Figure 8 where they are compared to the mean annual groundwater abstracted volume of groundwater for the period 2003–2018. It is clear that the groundwater abstractions form a significant portion of the water balance (circa 25% of the median annual recharge) and will reduce baseflow in the local streams. It is difficult to validate the long-term water balance in the absence of continuous streamflow gauging. However, infrequent spot gauging provided estimates of average discharge of 0.067 m<sup>3</sup>/s and 0.058 m<sup>3</sup>/s at two small streams, which are of the same order of magnitude as simulated average surface runoff at those locations (0.032 m<sup>3</sup>/s and 0.023m<sup>3</sup>/s, respectively).

Details of the long-term groundwater balance can be found in Table 4. It should be borne in mind that these estimates are for the whole recharge model area, and, whereas all of the abstractions are from the Fell Sandstone, not all of the recharge will reach the Fell Sandstone. Therefore, the water balance is for an area larger than the groundwater abstractions obtain their inflow. The recharge produced by ZOODRM is potential recharge and doesn't take into account the distribution of the Fell sandstone outcrop, therefore that reaching the water table (actual recharge) is calculated within the groundwater flow model. There is a large amount of uncertainty in the estimation of outflow as baseflow/springs. The estimate was derived from the two spot gauging sites. Owing to the limited amount of data and the fact that groundwater heads are generally dominated by large inter-annual trends rather than seasonal fluctuations, annual baseflow was estimated as the annual minimum gauged flow. The long-term average baseflow/spring flow was then defined as the median annual baseflow and assumed to be constant across the whole model area. The two sub-catchments associated with the spot gauging sites comprise 33% of the total area and 45% of the Fell Sandstone outcrop area of the recharge model area. Inflow/outflow from/to other groundwater units was assumed zero because of a lack of information. However this assumption may lead to water lost or gained from the aquifer, particularly from flow outside the model boundary, but also from the Scremerston or the Ballagan.

### 4.3 Simulated groundwater heads and budget.

The optimal values for the input parameters estimated after calibration of the MODFLOW model are presented in Table 5. According to the calibrated hydraulic conductivity and thickness values of the sandstone units at the borehole locations, the following transmissivity values were estimated:

- 18.6 m<sup>2</sup>/d at Borehole A (Layer 1, South Ord Sandstone)
- 15.5 m<sup>2</sup>/d at Borehole B (Layer 2, Murton Craggs Sandstone)
- 46.2 m<sup>2</sup>/d at Borehole C (Layer 4, Peel Knowe Sandstone)
- 46.7 m<sup>2</sup>/d at Borehole D (Layer 4, Peel Knowe Sandstone)
- 42.0 m<sup>2</sup>/d at Borehole E (Layer 2, Murton Craggs Sandstone)
- 35.5 m<sup>2</sup>/d at Borehole F (Layer 2, Murton Craggs Sandstone)

Whilst these are different from those derived from pumping test analyses, they are consistent with the lower end of the range of transmissivities reported in the literature. It is, however, to be noted that pumping tests analyses have a large degree of uncertainty associated with them related to measurement errors, design of test, availability of observation boreholes and its interpretation. Therefore, they are treated as guide values for groundwater modelling as they rarely produce transmissivity values that can be placed directly into a regional model.

Simulated and measured hydraulic heads for 18 observation boreholes are compared in Figure 9. Simulated heads reasonably match the measured values at the pumping stations (Figure 1; A-C, E and F) and at most of the observation boreholes. It is, however, to be noted that the accuracy of the time series data improves after 2011, due to increased use of manual dips to correct any drift in the transducers used for groundwater head measurement in the boreholes. For the boreholes in the Peel Knowe sandstone unit (i.e. Peel Knowe, Thornton Farm, and Shoreswood Loan) the model correctly reproduces the decreasing head trend observed in the 1990s, although groundwater heads are overestimated. This discrepancy could be the result of unaccounted for private groundwater abstractions from local farms or an oversimplification of the geometry of this sandstone unit in the model. In the current geological interpretation, Peel Knowe seems to consist of three individual subunits which were integrated into a single layer in the model. The model accuracy is poor (root mean square error RMSE > 10 m, see Table 6) for the observation boreholes in the Peel Knowe, those at The Kells, Murton Dean, Thornton Mains OBH, and Murton Craggy Bog. It is worth noting that measured groundwater heads in The Kells borehole displays a



unique upward trend and levelling off, for which neither the conceptual model nor the numerical model can provide a reason. Similarly, data from the Murton Craggy Bog borehole present a sudden variability that could be possibly linked to episodes of very high precipitation. Further, the time discretisation into monthly recharge periods is not particularly suitable for reproducing such sudden intense recharge episodes. The mismatch between observed and simulated data at Borehole B could be related to the uncertainty in the geological interpretation at this borehole, which shows the coalescence of the two upper sandstone units and a thick mudstone unit unrelated to any of the other units considered in the model (see Table 4). Other reasons include but are not limited to erroneous pumping data since the modelled hydrograph does not follow the behaviour of the observed hydrograph with respect to sudden changes in the pumping rate over time.

Overall, the mismatch between simulated and measured values measured in term of RMSE is equal to 8.8 m. However, when the most problematic boreholes (i.e. the bottom four in Table 6) were excluded from the analysis of the residuals, the average RMSE falls to a value around 4.5 m. This value is considered an acceptable margin of error considering the complexity of the aquifer system and the uncertainty in the interpretation. In particular, the main sources of uncertainty are the geometry and continuity of the sandstone and mudstone units in certain areas of the model domain, the lack of data for the definition of the boundary and initial conditions, particularly the lack of knowledge regarding the natural initial state of the flow field predating the abstractions.

Model estimates of the groundwater budget are presented in Figure 10. Over the simulated period (30 years), the total abstracted groundwater volume (62,634 MI) is about 7% lower than the cumulative recharge (67,228 MI). This discrepancy shows that to balance the model water balance, inflow is required from across the boundary via the GHB and that the size of the model may need to be increased. However, the recharge water balance (see Figure 8) does show the LTA flows to be in surplus with respect to abstraction. The difference between Figure 10 (groundwater model balance) and Figure 8 is related to the area covered with the recharge model having a larger geographic area whilst retaining the same groundwater abstractions from the Fell sandstone.

## 5 Conclusions

This paper presents new geological and hydrogeological interpretation of the Fell Sandstone aquifer in the area near Berwick-upon-Tweed. This knowledge has been encapsulated into a multi-layered numerical groundwater flow model and the conceptual understanding tested. The sustainability of supply from the groundwater system has been investigated.

The main findings from the work are as follows:

- (1) The system is complex, with variation in spatial interactions between the sandstone units. There is a need to conceptualise the system as seven discrete sandstone units, unusually for a British aquifer and its associated groundwater system, particularly of this size. The interaction of different sandstone units vertically can be important. Generally, they are separated by very low K mudstone units. However, this relationship changes spatially and certain sandstone units, namely Murton Dean and Royalty, have limited extents as well as direct interconnection in places.
- (2) Differing time responses between variations in the hydraulic stresses (i.e. recharge or abstractions) and the resulting changes in groundwater heads exist. There are also differences in temporal response between units with a general slow accumulation of recharge (accumulating over six months). However, some hydrographs show very rapid response, e.g. Murton Craggy Bog which can see a response to storm events (Dearlove et al., 2022). Other boreholes such as The Kells demonstrate a very unusual groundwater response which requires further investigation.
- (3) The geology and hydrogeology of the Fell Sandstone is complex, with significant vertical and lateral interactions in a small area. Whilst the Scremerston overlays the Fell Sandstone and is considered as a non-aquifer, there remain questions as to its behaviour. One of these is how permeable its lower formation is and, in particular, whether this horizon produces inflow to borehole A.

Despite the recent investigations, there are uncertainties that could be reduced through further study: including the 3D geometry of the units; the further delineation and investigation of the role of the faults; stream–aquifer interactions; and a water balance for the whole area. The next planned phase of work is to widen the area of interest both toward Berwick and further south-west. This will take the form of combined geological–hydrogeological fieldwork alongside groundwater modelling. It is expected that, by continually iterating the geological and numerical models along with the conceptual understanding of groundwater flow to address particular questions in specific locations, an holistic understanding can be formed to assist both the water company in its exploitation of the aquifer and the regulator in its oversight.

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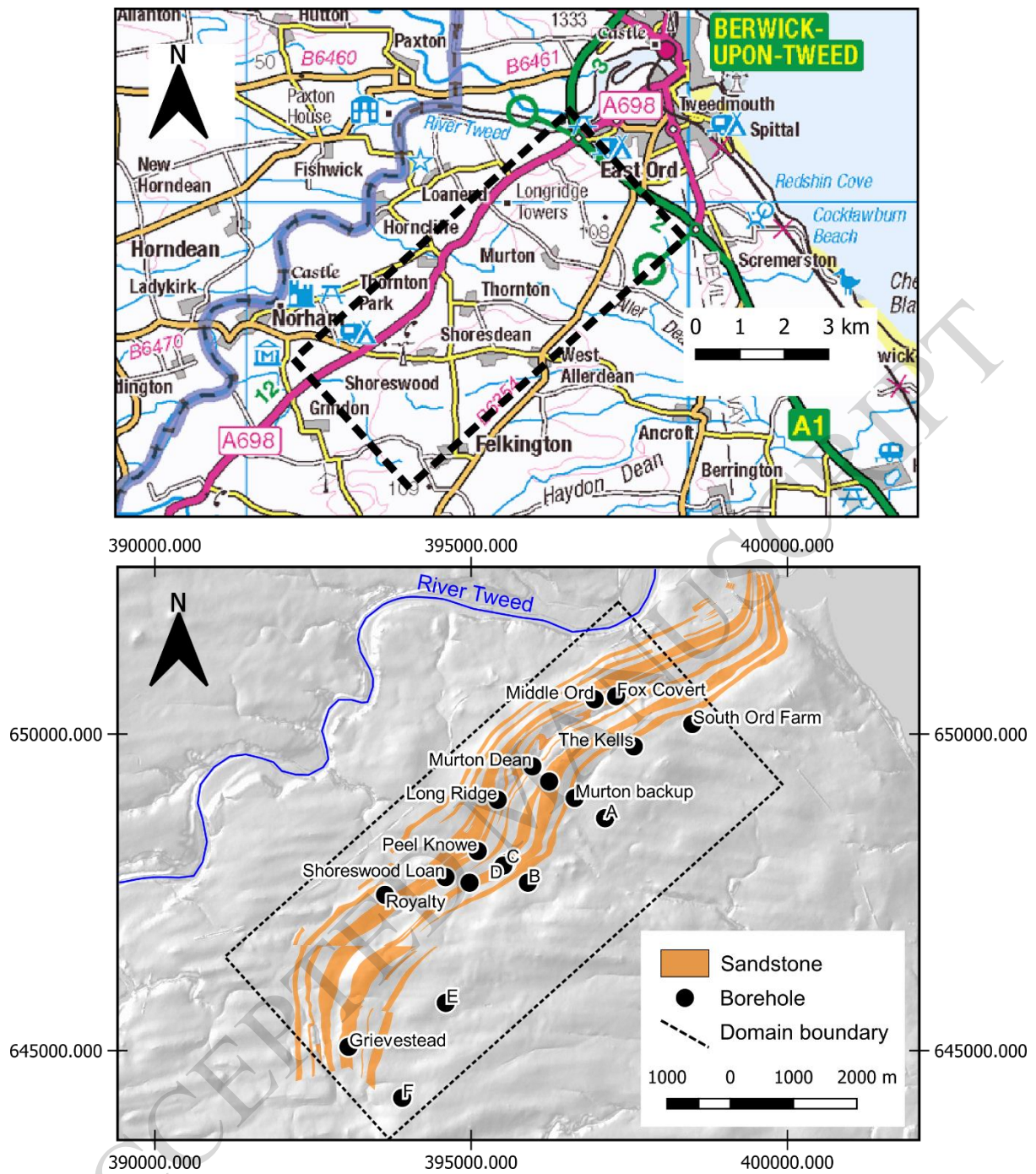
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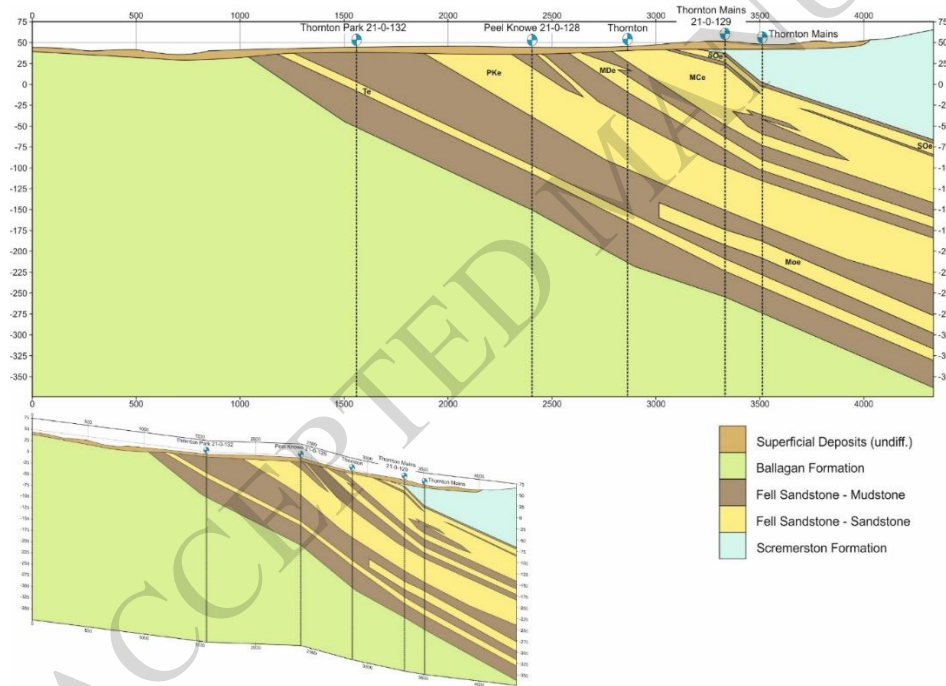
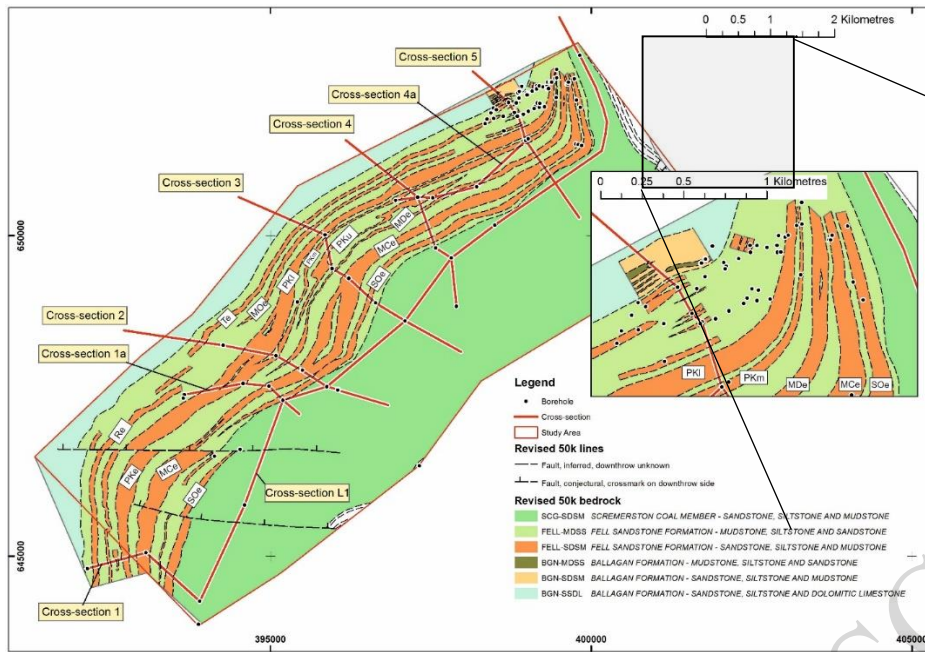
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**Figure 1. Location of the study area. The dashed line represents the boundary of the numerical model grid. Borehole locations are also shown. Geological outcrop of the Fell Sandstone is denoted in orange. OS Open Data © Crown Copyright.**



**Figure 2. (a) Geological outcrop of the Fell Sandstone. Insert map covers the area around Berwick-upon-Tweed with axis of the anticline shown as dashed black line (b) cross-section no. 2**



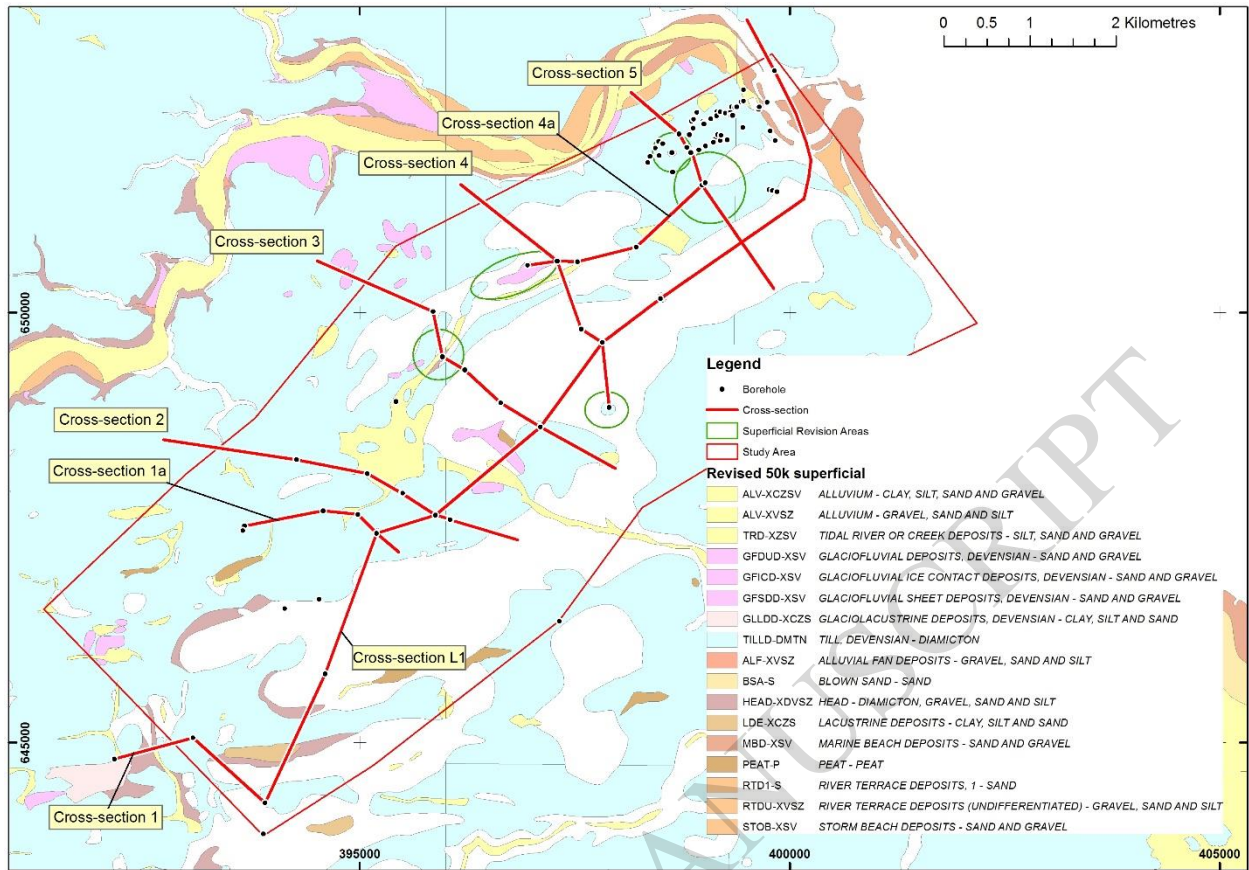
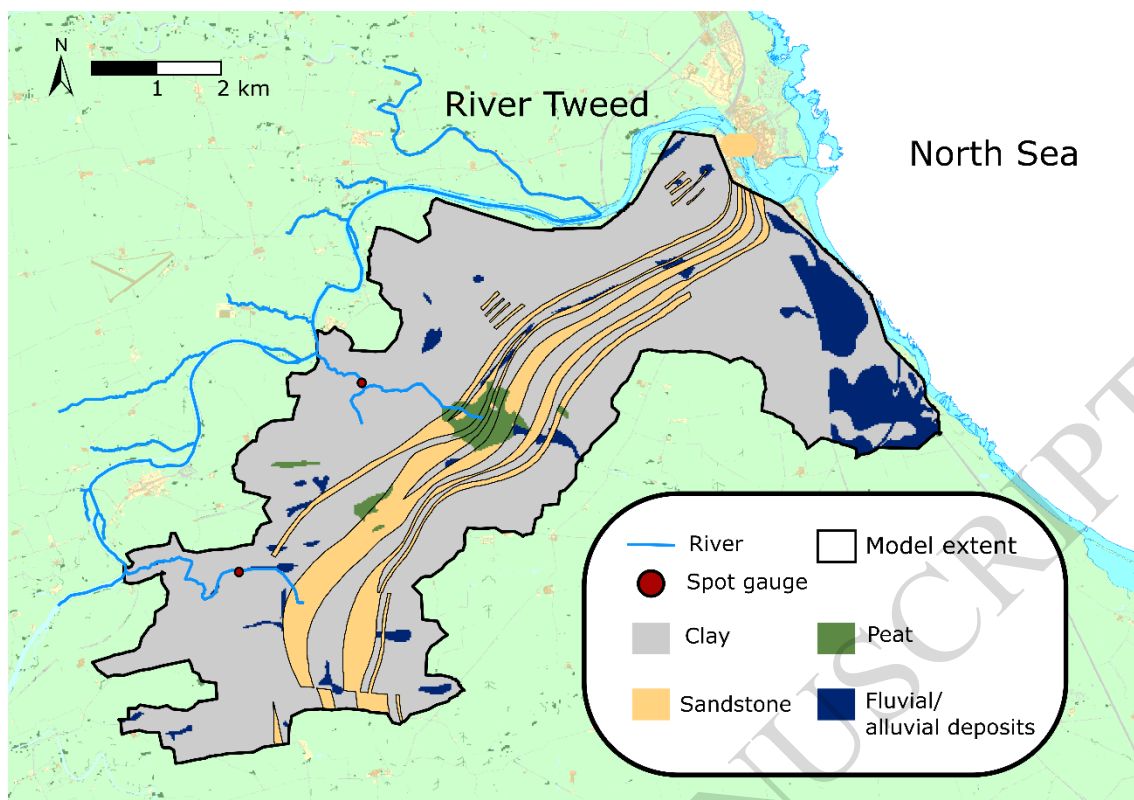
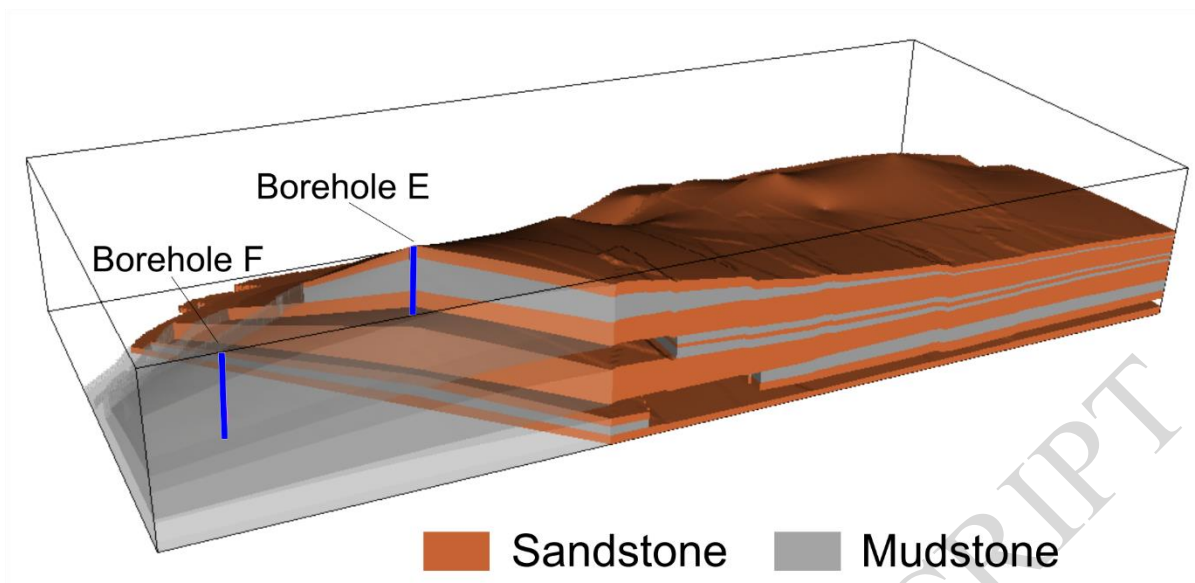


Figure 3. Superficial geology over the study area.

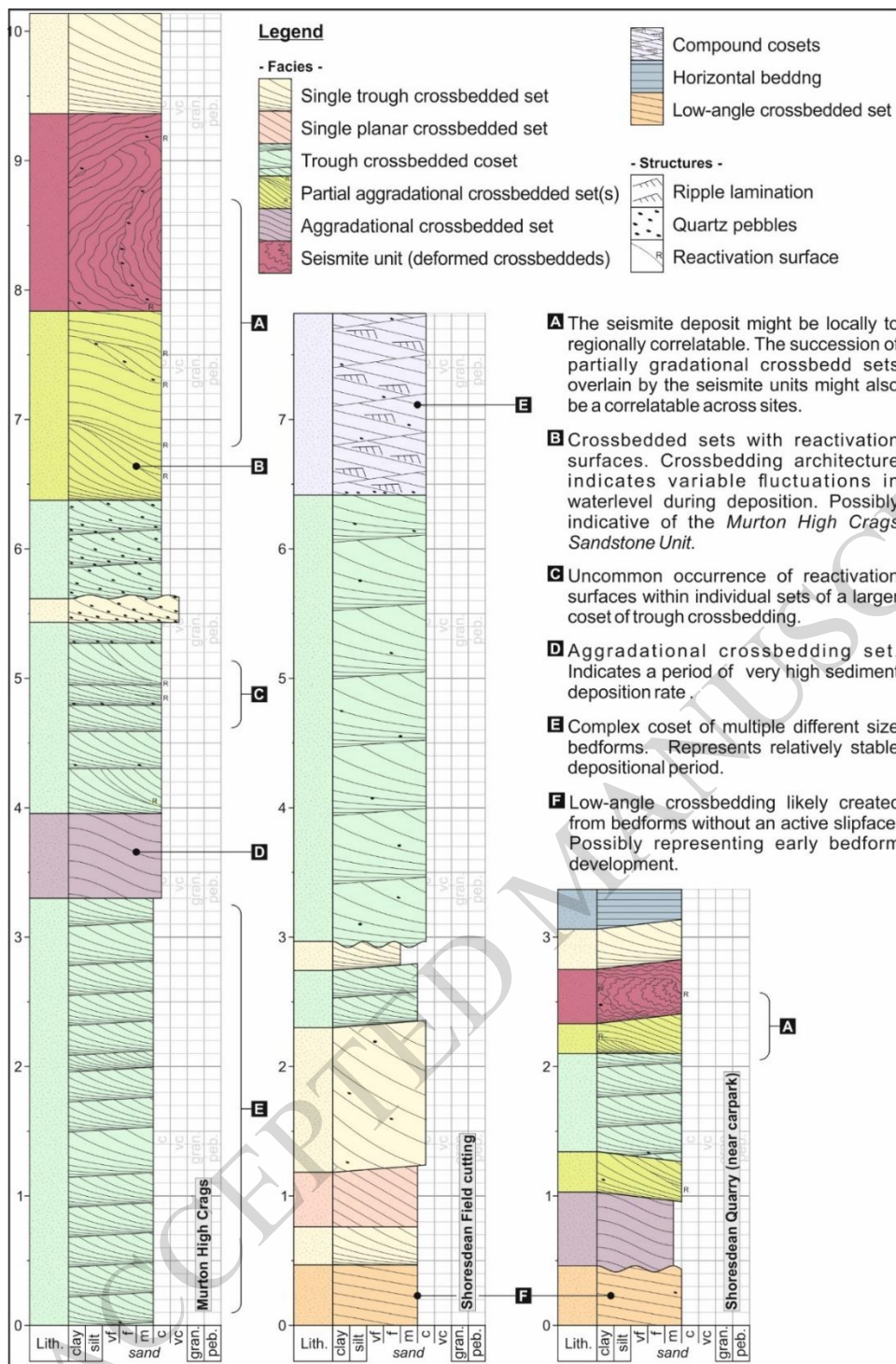


**Figure 4. Recharge model extent and soil description, based on BGS Parent Materials (Lawley 2011). OS Open Data © Crown Copyright.**



**Figure 5. Cut-out diagram showing the model construction with the Fell Sandstone layers (red-brown) interspersed with Mudstones (grey). The abstraction boreholes are shown as vertical “sticks”.**

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**Figure 6. Sedimentary Logs constructed from field outcrops at Murton High Craggs, and Shoreswood**

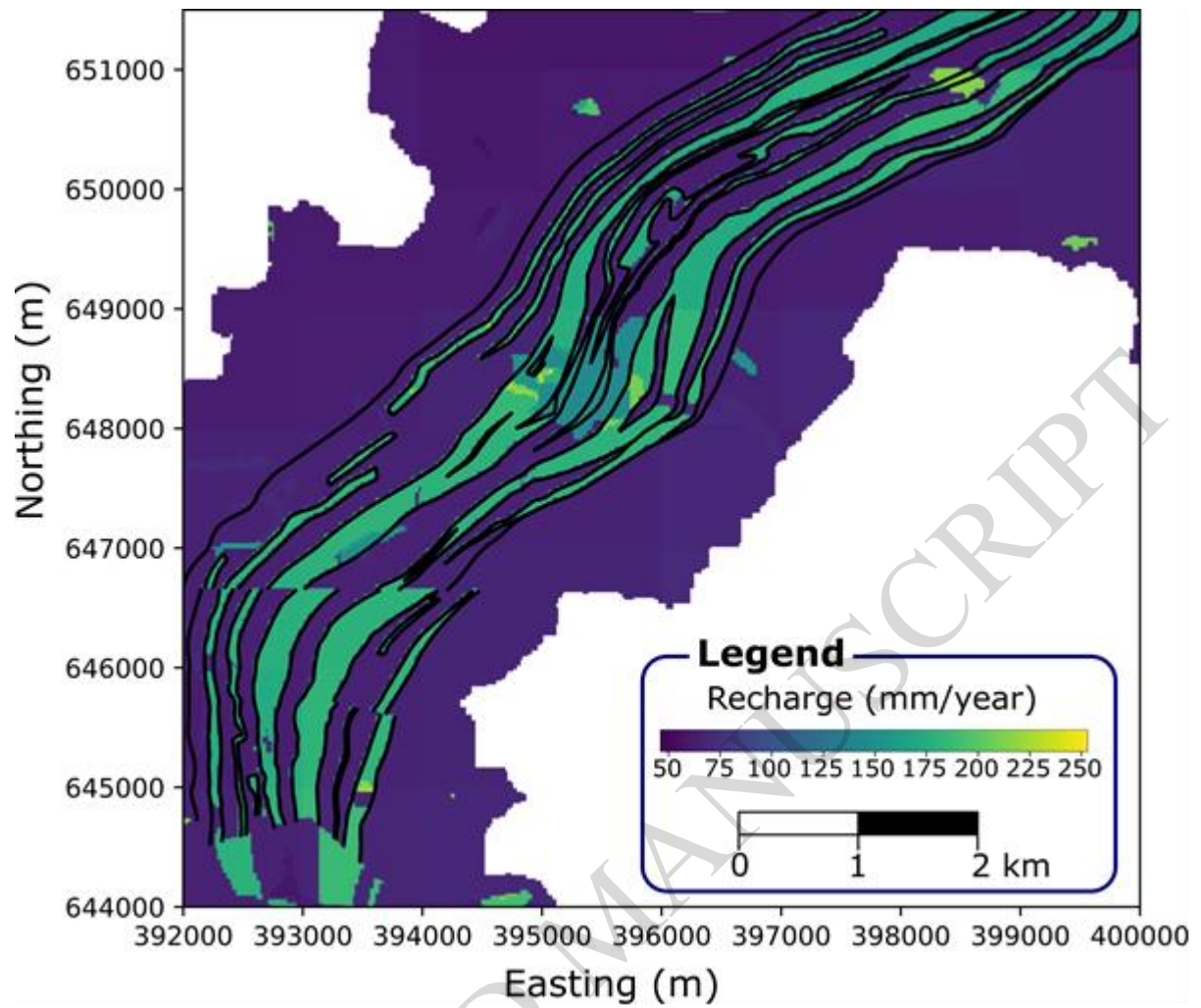
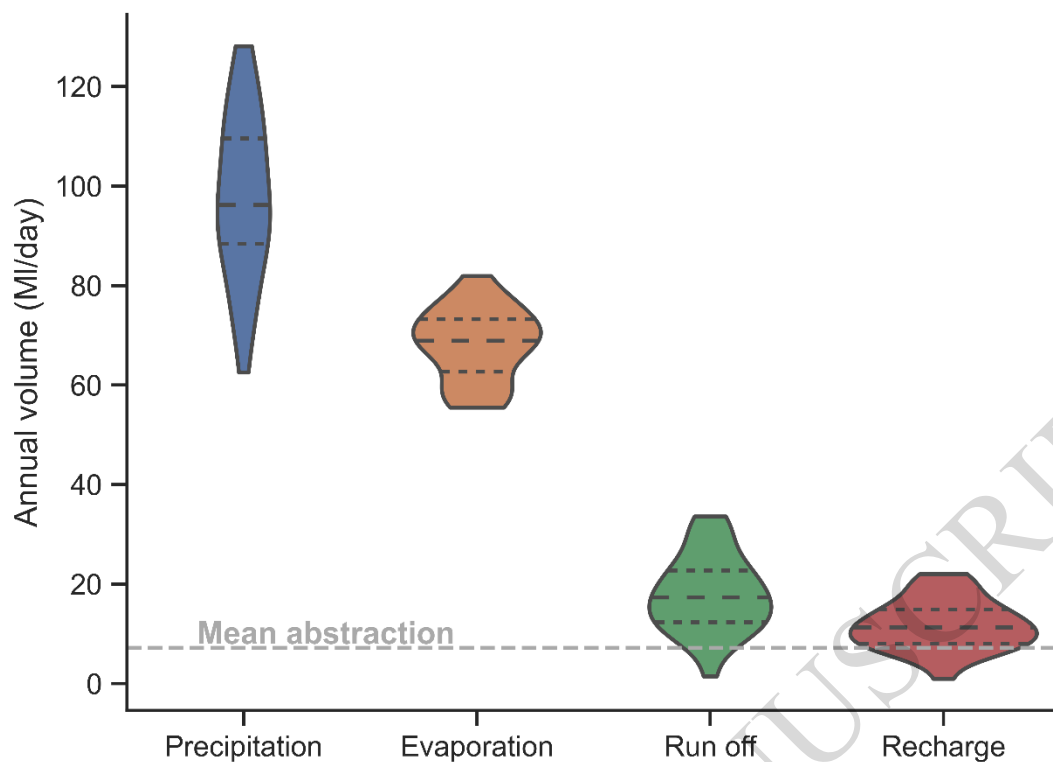


Figure 7. Distributed long-term average recharge (mm/a).



**Figure 8. Water balance from recharge model 1988–2018. Mean abstraction (grey dashed line) is for the period 2003–2018. The shape represents a kernel density estimation of the underlying distribution with the large dashed line representing the median (50% quartile) and smaller dashes the 25% and 75% quartiles.**

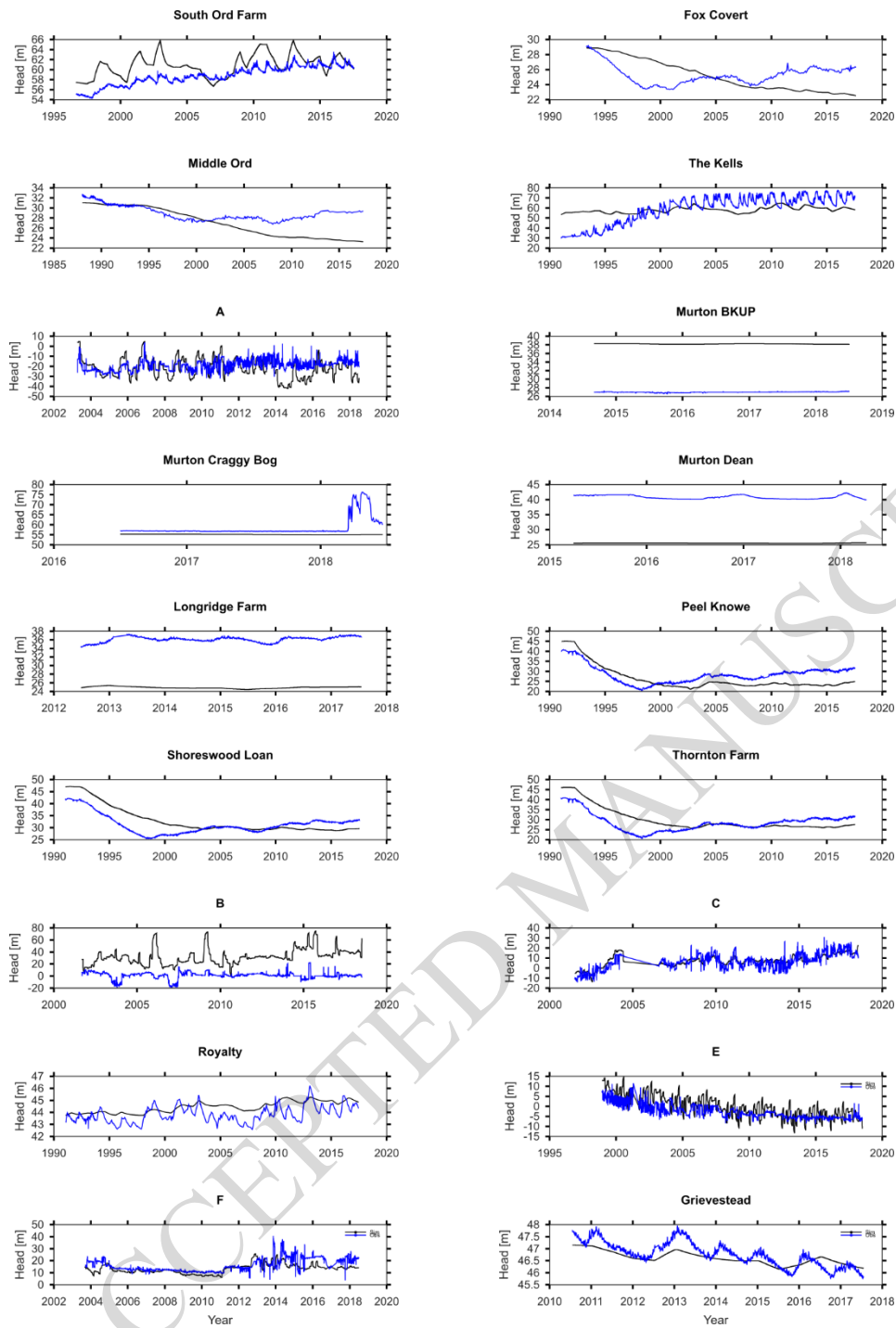
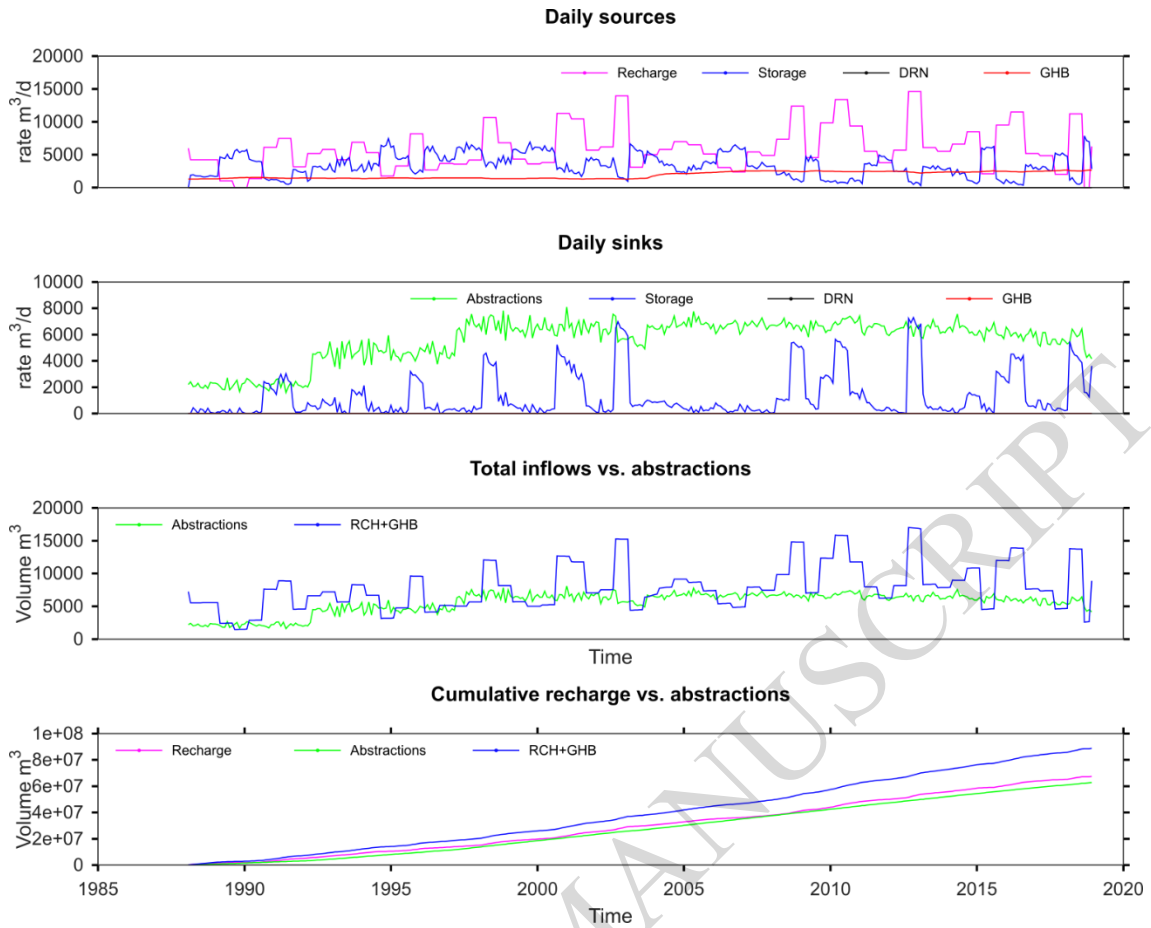


Figure 9. Simulated (in black) vs measured (in blue) groundwater hydrographs.



**Figure 10. Simulated groundwater budget. DRN, drainage to springs/outflows; GHB, general head boundaries representing groundwater inflows/outflows; RCH, recharge.**



**Table 1 - Principal data sources for geological understanding**

<b>Type</b>	<b>Source</b>
<b>Digital elevation models</b>	NextMap (5 m cell-size) digital surface and digital terrain models; EA IHM (Integrated Height Model) 2017 2 m resolution digital terrain model (DTM); BGS Bald-Earth DTM (5 m cell-size)
<b>Topographic data</b>	Various scales of modern Ordnance Survey data
<b>Digital aerial photography</b>	Sourced via the Pan Government Agreement
<b>Existing geological map data</b>	Published BGS 1:50,000-scale digital geological map data
<b>Historical geological fieldslips</b>	Scanned and georectified BGS fieldslips related to the primary geological survey of the district dated 1890-1930
<b>Maps and reports provided by the EA and NWL</b>	Various geological map and cross-section interpretations for the Fell Sandstone
<b>Borehole data</b>	Borehole records obtained from the BGS National Geoscience Data centre, plus additional data supplied directly by the EA and NWL
<b>Recent geological field data</b>	Digital geological data acquired as part of this study in the southern part of the study area (indicated on Figure 1)

**Table 2 - Data requirements for recharge model**

<b>Data requirement</b>	<b>Dataset</b>
Precipitation	GEAR rainfall up to end of 2015 (Keller et al., 2015). 2016–2018 UK EA gridded data
Potential evapotranspiration	MORECS potential evapotranspiration
Soil data – field capacity, wilting point and rooting depth	HOST (Boorman et al 1995)
Runoff coefficients	BGS Parent materials ((Lawley, 2014) / BFIHOST
Land cover data	LCM2007 (Morton et al., 2011)
Stream flow data	Two infrequent EA spot gauges
Digital terrain model	10 m NEXTMap

BFIHOST – Estimate of the base flow index (BFI) based on the Hydrology of Soil Types (HOST) classification; EA: Environment Agency; GEAR – Gridded estimates of daily and monthly areal rainfall for the United Kingdom; LCM2007: Land Cover Map 2007; MORECS, Meteorological Office Rainfall and Evaporation Calculation System.

**Table 3 - Generalised succession of the main sandstone layers shown in the study area; thin, laterally impersistent sandstone units not shown**

BGS Revised interpretation (Tentative correlation with Turner et al. 1993 where appropriate)		Comments		
<b>Scremerston Formation</b>				
Fell Sandstone Formation		Mudstone	Locally absent	
		South Ord equivalent	10-15 m thick. Locally absent	
		Mudstone (locally absent)	Locally absent. Not present just east of Thornton.	
		Murton Crag equivalent; includes mudstone partings	Relatively thickness variations from 20 – 50 m. NB. Inferred considerable thickness change around Shoreswood is poorly constrained. Directly underlies South Ord equivalent in places.	
		Mudstone	Relatively persistent.	
		Murton Dean equivalent	5-20 m. Poorly constrained and possibly absent in the south of the study area	
		Mudstone	Relatively variable thickness, 5-15 m?	
	Peel Knowe equivalent (undivided)		Peel Knowe equivalent upper leaf	10-20 m Present in the central part of the study area.
			Mudstone	Highly variable unit. Appears to form as both interleaving mudstone between upper and middle Peel Knowe leaf equivalents and also as isolated mudstone lenses within the Peel Knowe where the leafs conflate.
			Peel Knowe equivalent middle leaf	Thickness is hard to define (up to 40m?), as it appear to merge with lower Peel Knowe leaf frequently.
			Mudstone	Highly variable unit. Appears to form as both interleaving mudstone between upper and middle Peel Knowe leaf equivalents and also as isolated mudstone lenses within the Peel Knowe where the leafs conflate.
			Peel Knowe equivalent lower leaf; includes mudstone partings	Likely the thinnest of the Peel Knowe leafs; thickness (5-15m? Conflates with lower leaf in the southern part of the study area
			Mudstone	Absent in the southern part of the study area

	Middle Ord equivalent	5-10 m thick. Recognised in the central and northern parts of the study area
	Mudstone	Relatively lateral persistent mudstone unit. Thickness likely >15 m
	Royalty Sandstone equivalent	Recognised in the southern part of the study area. Thickness varies up to about 20 m
	Mudstone	Relatively lateral persistent mudstone unit. Thickness about 15 m
	Thornton Park equivalent	Very poorly constrained, with little borehole evidence. Thickness ~10m? Recognised in the central and northern parts of the study area
	Mudstone	Relatively lateral persistent mudstone unit. Thickness likely at least 10 m
<b>Ballagan Formation</b>		

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**Table 4. Long-term average (1988–2017) groundwater balance**

	<b>Components</b>	<b>Volumetric Flow rate MI/day</b>	<b>Equivalent recharge rate (mm/a)</b>
Inflow	Potential recharge (direct and indirect)	11.7	80.5
	Inflow from other groundwater units	0	0
Outflow	Abstraction	6.56	45.2
	Baseflow/springs	2.6	17.9
	Outflow to other groundwater units	0	0

**Table 5. Calibrated model parameters**

Model Layer	Fell SDST formation name	Horizontal conductivity (K) of sandstone layers at outcrop [m/d]	Vertical K of confining layers (mudstone units) below sandstone units [m/d]	Storage coefficient (S) at outcrop [-]
1	South Ord	1.9	2.0e-04	6.0e-02
2	Murton Crag	3.4	5.0e-04	6.0e-02
3	Murton Dean,	2.0	5.0e-05	1.0e-02
4	Peel Knowe	0.8	5.0e-05	6.0e-02
5	Middle Ord	1.1	5.0e-03	1.0e-02
6	Royalty	5.0	1.0e-02	1.0e-02
7	Thornton Park	5.0	5.0e-03	5.0e-03

**Table 6. Calculated RMSE values for the calibration boreholes**

<b>Borehole</b>	<b>RMSE (m)</b>
Greavestead	0.353
Royalty	1.56
Middle Ord	2.613
Borehole E	2.997
Borehole F	3.556
Fox Covert	3.675
Peel Knowe	4.106
Long Ridge	5.27
Murton Backup	5.342
South Ord Farm	6.216
Thornton Farm	6.392
Borehole C	6.657
Borehole A	6.972
Shoreswood Loan	7.192
Murton Dean	10.27
Borehole B	16.426
Murton Craggy Bog	19.383
The Kells	22.091