RIGOROUS 3D GEOLOGICAL MODELS AS THE BASIS FOR GROUNDWATER MODELLING

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1. INTRODUCTION AND BACKGROUND

Increasing environmental pressures, pollution and legislation in Europe are creating the urgent need for regional-catchment scale geological models to assess hydrogeological conditions and inform mathematical and numerical groundwater models. Geological models are especially important in areas with superficial deposits overlying key aquifers. These areas are often characterized by very complex arrangements of aquifers and aquitards, having important implications for aquifer protection, flow pathways and recharge potential. The interaction of ground and surface water in valleys is being closely studied following many recent instances of inundation in Europe.

In the past, 2 dimensional datasets, such as geological maps and cross-sections, were used in coordination with site-specific point data to build a conceptual understanding at the site or catchment scale. A simplified version of the conceptual understanding and geological structure would then form the framework for groundwater flow modelling. Robins et al (2005) identified that it is essential that the geological framework and conceptual groundwater model should be considered together in order to avoid loss of understanding of the geological structure and its relation to the hydrogeology. In essence the over-simplification of geological structure in groundwater models can lead to unrealistic results and unreliable modelling outputs.

The technology behind current groundwater modelling codes has been unchanged for over 20 years. The USGS groundwater flow code MODFLOW is a prime example. The main drawback with these codes is that they are not easy to change as they are coded in procedural languages such as FORTRAN. The computer programming community has adopted object-oriented (OO) techniques for widespread use due to the flexibility, re-usability and the ease of code maintenance offered. OO technology is now mature and is widely used and the advantages of OO technology can be exploited to develop groundwater model codes.

BGS is currently building systematic 3D geological models of the shallow subsurface, and in particular superficial deposits, using the GSI3D software and methodology (Kessler and Mathers 2004). These models are being structured and attributed to meet the needs of a wide range of applied users with many models already built for diverse commercial clients in the UK including the Environment Agency of England and Wales, water and utility companies, local Government, and the Archaeology-Heritage sector. A key functionality of the software used to build the 3D geological models (GSI3D) is that it is compatible with our bespoke groundwater modelling software (ZOOM). So the geological sediment body geometry can be directly imported into the ZOOM software to give a realistic geological framework for groundwater flow modelling.

This paper summarises our methodology for 3D geological modelling and groundwater flow modelling, and importantly how the two preferred software packages interact. We also describe case studies where geological models have contributed significantly to hydrogeological understanding.

2. THE GSI3D METHODOLOGY

The GSI3D software tool and methodology has been developed over the last 15 years and since 2001 in cooperation with the BGS. The GSI3D philosophy and workflow are described by Kessler and Mathers (2004) and also Merritt et al (2007). The success of the GSI3D methodology and software is based on its intuitive design and the fact that it utilizes exactly the same data and methods, albeit in digital forms, that geologists have been using for two centuries in order to make geological maps and cross-sections. The geologist constructs models based on a career of observation and the feeling that something "looks right to a geologist" and so incorporating tacit knowledge, is a key element in the GSI3D approach.

GSI3D combines Digital Terrain Model, geological map and downhole borehole data to construct regularly spaced intersecting cross sections by correlating boreholes and the outcrops-subcrops of units to produce geological fence diagrams. Mathematically interpolating between the nodes along these sections (and the

outcrop/subcrop limits of the units) produces a solid model. This is built from a series of stacked triangulated objects, each corresponding to one of the geological units present.



Figure 1. Flowchart showing process of developing a numerical model from basic data using both visualisation and conceptualisation, from Robins et al. (2005)

The result of the modelling is a representation of the subsurface taking into account all available surface and subsurface data and incorporating the conceptual understanding of the survey geologist.

3. THE ZOOM FAMILY OF MODELS

The ZOOM family of numerical groundwater models consists of the saturated groundwater flow model ZOOMQ3D (Jackson and Spink, 2004), the advective transport particle tracking code ZOOPT (Jackson, 2004) and the distributed recharge model ZOODRM (Mansour and Hughes, 2004). All of these models can be created using a pre-processor called ZETUP (Jackson and Spink, 2004). Each of these models has been developed using object-oriented techniques, a programming approach commonly applied in commercial software development but only relatively recently adopted in numerical modelling for scientific analysis. The main feature of the ZOOM models is grid refinement so that any numbers of linked finite-difference grids can used to literally zoom in on a particular part of the groundwater system.

The ZOOM family of models has been used extensively and their use reported in the literature. Examples of the use of the flow model ZOOMQ3D include a regional model to the southeast of London (Jackson et al., 2003), a model to examine abstraction from the Goring Gap section of the Thames Valley, (Jackson et al., 2007), and a basin scale model in Scotland, (Jackson et al., 2003). A flow model has also been used in conjunction with the particle tracking code, ZOOPT, to examine pesticide movement in the Permo-Triassic Sandstone in Yorkshire (Stuart et al., 2006), whilst a recharge model, ZOODRM, has been applied to the West Bank, Palestine (Hughes et al., in press, Hughes et al., 2006).

4. THE GSI3D – ZOOM INTERFACE

An interface between the groundwater flow model ZOOMQ3D and GSI3D has been developed. A ZOOM grid is imported in to GSI3D and the values for top and bottom of each layer as well as the hydraulic properties of the layer are exported from GSI3D. The stratigraphic sequence file in GSI3D is attributed by the user to allow the hydrogeological units to be identified from the geological units. The ZOOM setup program, ZETUP has been modified to accept the data from GSI3D and to create the input files for ZOOM in the correct format. The whole process is no more difficult than setting up a ZOOM model using a GIS.



Figure 2. Revised flowchart showing integration of geological and conceptual groundwater model.

The coupling of the geological and conceptual groundwater model within GSI3D and the direct export of attributed geological objects and their geometries ensures a dynamic link is maintained throughout the workflow. It is envisaged that in the future the numerical models will also inform the geological model.

5. EXAMPLES OF THE APPLICATION OF GEOLOGICAL MODELS

5.1 The Oxford groundwater flooding study

The City of Oxford is situated within the narrow valley of the Thames and is underlain by alluvial deposits comprising alluvium and river terrace deposits. The city suffers from recurrent floods caused by high groundwater levels and over-banking of the floodplain of the Thames and its tributaries (Macdonald et al., 2007). A GSI3D geological model has been developed for the superficial deposits in this area.

This model forms the basis of a ZOOMQ3D groundwater flow model. A dense groundwater level monitoring network of over 100 piezometers has been used to create groundwater level contour maps for the area. These contour maps have been combined with the 3-D geological model to allow the potential storage within the unsaturated zone under the floodplain to be assessed. The model defines two units: the near-surface silty, clayey alluvium (around 1 m thick) and the underlying sand and gravels (on average 5 m thick). Combining groundwater levels with the 3-D model allows the volumes of unsaturated alluvium and sands and gravels to be estimated. Assigning storage coefficients to these units gives an indication of the relatively small volumes of infiltrating water that are required to bring groundwater levels to the surface causing groundwater flooding. For example, for a typical spring the volume of unsaturated zone storage is in the order of one day of high flow in the River Thames.

5.2 The Goring Gap study

Groundwater models of UK aquifers are usually developed to investigate regional water resources and to aid their management. There are, however, many instances of them being applied subsequently to problems and scales for which they were not originally intended. To apply models at different spatial and temporal scales a range of data should be used to develop appropriate conceptual models and to validate the resulting numerical model. In the Goring Gap the Thames flows south-eastwards through a narrow gorge to enter the London Basin. Here geological modelling, hydrogeochemical sampling, borehole and surface geophysics and pump testing have all been used to improve the representation of the aquifer within the ZOOMQ3D regional finite-difference groundwater model.

The flow model is used to assess the provenance of groundwater abstracted from a major public supply well in a regional aquifer and to check the sustainability of increased abstraction. The boreholes are located adjacent to the River Thames and derive their water from a combination of the river, the underlying terrace gravels and the regional Chalk bedrock aquifer. Consequently, conceptual and numerical models are required from the site- to the regional-scale.

At the site-scale a range of information has been collected and interpreted in order to develop detailed conceptual and numerical models. A geological model of the sub-alluvial sand and gravels (Figure 4) and the underlying Chalk has been constructed using GSI3D. Geological units can be attributed as hydrogeological units within GSI3D and their resulting geometry and hydraulic properties exported directly to ZOOMQ3D. This enables a significantly improved representation of the hydrogeologically important superficial deposits to be included in the numerical flow model.



Figure 3. The GSI3D model of the superficial deposits in and around the floodplain of the River Thames in the Oxford area (made ground – pink; alluvium – yellow; terrace and sub-alluvial sands and gravels – orange) and the contoured water table in mauve.



Figure 4. GSI3D geological model of the geometry of the sub-alluvial sands and gravels of the River Thames in a 10 x 10 km area around Gatehampton in the Goring Gap.

6. OUTLOOK

Experience will be built up using GSI3D to produce ZOOM models. The aim is to incorporate a GSI3D model into any groundwater modelling project. The geological model will be seamlessly transferred to a groundwater flow model once the hydrogeological units have been identified. It is envisaged that interaction will take place routinely between the geologists who produce the GSI3D model and the hydrogeologists who create the groundwater flow model. This iterative process will inform and develop both the geological and hydrogeological understanding of the system under study.

The ultimate aim of the use of GSI3D is to provide a proper representation of geology to enable the development of a better conceptual understanding of groundwater flow and, subsequently, an appropriate groundwater model. It has become apparent from the use of 3D geological modelling that the representation of geological units as layers in groundwater flow models has its limitations. From the Goring Gap study described above, it can be seen that geological and hydrogeological units are not continuous layers, but are discrete volumes. Therefore, a groundwater modelling system has to be developed that better represents geological complexity.

A further vision is to develop viewing tools that can be used to deliver these visualisations and model results to customers. These viewers must be able to run on standard PCs and they have to be easy to use, so that the results of the modelling work can be accessed by everyone including customers, government departments and the general public.

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