Matching Groundwater Flow Models

Adriana Moreno[1], Tim Atkinson[2] and Richard Simons[3]
Departments of Civil & Environmental Engineering and of Earth Sciences, UCL
a.moreno@ucl.ac.uk[1]; t.atkinson@ucl.ac.uk[2]; r.r.simons@ucl.ac.uk[3]

ABSTRACT: This paper describes the matching of two groundwater flow models based on Finite Difference (FD) and Finite Element (FE) codes. The work has been carried out as part of a wider study of transport in fractured chalks, in which basic hydrological data are required to drive a finite-difference local scale model. A regional-scale FD groundwater flow model using the MODFLOW code has been developed to simulate existing flow conditions around a case study area in North West Norfolk, England. This model has been built using controlling parameters shared with an FE flow model in AQUA-3D developed by AWG (1997) to evaluate the groundwater flow rates. Comparison between the models was made on the basis of the flow and head fields in the chalk aquifer which is of particular interest in the wider research study.

Keywords: numerical groundwater models, Chalk aquifer, MODFLOW and AQUA-3D.

1. Introduction

Numerical models of groundwater flow have been used since the late 1960s to represent the hydrogeological features seen in the field. For example using a groundwater model, it is possible to test various management schemes and to predict the effects of certain actions.

This work considers two types of models – first using the Finite Difference (FD) MODFLOW code and second using a Finite Element (FE) code, AQUA-3D. Both use a system of nodal points superimposed over the problem domain. In MODFLOW the FD method is implemented with rectangular cells, whilst in AQUA-3D the FE method is implemented with a variety of element types such as triangles defined by three nodes – one at each corner.

The purpose of the present paper is to describe how we matched two models based on these different approaches and examined them for equivalence in terms of predicted head and flow fields when each was based on the same set of parameters and steady-state boundary conditions.

2. Modelling rationale

The context of this study was a wider exercise in developing a methodology for risk assessment of potential contamination of wells by particulates. This required a flexible *gridded* code that allows local transport parameters to be changed at will, perhaps stochastically. MODFLOW is a very commonly used FD code in such studies, as (a) its gridded structure is suitable, (b) it is widely employed as a standard modelling package, and (c) contaminant transport modules are available. Some MODFLOW formats, including the Groundwater Vistas package employed here, incorporate facilities for stochastic parameter alteration which make them useful for risk assessment.

The region in which the risk assessment study was to be carried out had already been the subject of a modelling project (AWG 1997) with the aim of providing a transient flow model for management of water resources in the three aquifers that are present. The result was a FE model based on the AQUA-3D code. To build upon this existing model (and especially to capitalise on the large amount of preparatory work which had been involved in data compilation, formulation of a conceptual model, plus development and calibration of a multi-layer FE model realisation) it was decided to construct a second model based on MODFLOW which would reproduce, as closely as possible, the AQUA-3D realisation.

This is a highly unconventional approach to model construction, but one that there should be few objections to in principle. Essentially, the new model was to be calibrated against the existing model, and was to share as many of its parameter values as possible, rather than to be constructed completely afresh and calibrated against field data. The operational reason for this approach was to ensure close water balance and flow field equivalence between both models, and to allow MODFLOW to be used for case studies in contaminant transport that would be difficult or clumsy to perform on AQUA-3D.

The AQUA-3D code is written for transient flow and must be driven by time-varying boundary values. In contrast, contaminant transport problems in MODFLOW must be represented using steady state flow fields. Thus, it was essential to create a steady state version of AQUA-3D, driven by "time series" composed of constant, average values and to "reproduce" it the MODFLOW format.

The exercise revealed some of the difficulties and problems which can arise when attempting to construct equivalent models based on radically different FE and FD approaches to numerical approximation of the groundwater flow equations. The purpose of this paper is to describe some of these problems and how they were overcome.

3. The study area

The study area covers approximately 952km² in the eastern part of the United Kingdom between latitudes 52°38' N and 52°59'N and longitudes 0°25'E and 0°50'E. Its western and northern boundaries are at the sea in the Wash and north Norfolk coast respectively. The eastern boundary lies along the groundwater divide of the Chalk aquifer, separating groundwater flow which is directed to rivers draining westwards and north (within the study area) from flow to rivers draining east. The southern boundary lies along the groundwater divide between two westwards draining rivers – the Nar (within the study area) and the River Wissey. (BGS, 1994).

The area is characterized by very flat geographical features with its highest elevation of approximately 120m OD at ground surface. In general the topographic surface rises from close to sea level in the west to highest elevations along the eastern boundary. This west-facing regional slope is a muted escarpment, flattened by glacial erosion during the Pleistocene, and underlain by a series of Upper Jurassic and Cretaceous rocks which dip very gently to the east and contain three distinct aquifer units. The regional slope is dissected by a series of westwards draining rivers, with valley floors descending to around 3 m OD in the west. (Funnel and Larwood, 1970).

The geological succession commences in the west with the oldest strata which are Upper Jurassic clays. These are succeeded by a sequence of Cretaceous sands which form the lowest two-aquifer units, separated by clay aquitards. The lowest aquifer comprises the Leziate Beds which are fine to medium unlithified sands. They are overlain by the Dersingham Clay which forms a regional aquitard beneath the second aquifer which is formed by the Carstone, a silica sandstone with a strong ferruginous cement. This in turn is succeeded in the north of the area by the Red Chalk, a distinctive red-coloured, nodular limestone. In the southern part of the area the Red Chalk is not present but its lateral equivalent is a clay, part of the Gault Clay formation that occurs widely over south-east England. It forms a second aquitard beneath the third and highest aquifer in the sequence, the Chalk. This is a fine-grained porous limestone, with well-developed fractures that account for the majority of its permeability at a field scale. (It is the possibility of bio-particles being transported through these fractures which provides the ultimate reason for this study).

This sequence of solid geological deposits is in turn covered in places by Quaternary materials. On the highest ground, in the east of the area, glacial tills overlie the Chalk and may develop up to 80m thick. These have low permeability and where they occur they reduce the infiltration of water to the Chalk aquifer. Most of the Chalk and lower aquifer outcrops are free of glacial drift cover, but they may be overlain by deposits of wind-blown sands which date from the latest Quaternary. Groundwater abstraction occurs at a number of wells and pumping stations for private and public water supplies. (Hiscock, 1991).

4. Conceptual model

There are three aquifers which extend over the whole area of 952 km^2. The Chalk, the Carstone and the Leziate Beds. They are separated by aquitards – the Dersingham Clay between the two lower aquifers and the Gault Clay and Red Chalk between the two upper aquifers. Although our major interest for risk assessment is in the Chalk, the AQUA-3D model includes all three aquifers for purposes of water resource management. Thus, we conceptualise the region as underlain by a 5-layer system of three aquifers and two semi-permeable aquitards. In places, glacial drift comprises a sixth, low-permeability layer which rests upon the Chalk and reduces infiltration and recharge.

The discharges from these aquifers occur to rivers where these flow in valleys across their outcrops. All of the rivers in the modelled area originate on the Chalk aquifer. The four rivers which drain westwards (Heacham, Babingley, Gaywood and Nar) and the R.Burn that drains northwards all rise at springs from the Chalk. They are augmented by other springs and seepage of groundwater as they cross the lower parts of the Chalk outcrop and then traverse the outcrops of the two lower aquifers. A sixth river, the Wensum, starts on areas of Chalk that are covered by glacial drift. Groundwater seepage leaves the Chalk and feeds the river where the Wensum valley is deep enough to cut wholly or partially through the glacial deposits. In some places, glacial gravels are present beneath the clay-rich tills, and these may form local aquifers and springs which also augment the flow of the river Wensum which leaves the modelled area via the eastern boundary. (Boar *et al.*, 1994).

The groundwater surface in the Chalk aquifer is mostly an unconfined water table, except in the east where confined conditions occur beneath some parts of the till cover. This indicates that recharge must occur through the till, as the aquifer is confined in places where the groundwater level is highest. Thus, the glacial deposits overlying the Chalk act as a leaky aquitard, allowing some recharge to pass into the aquifer beneath them. (Toynton, 1979).

The groundwater surface of the Chalk is highest in the east, and the eastern boundary of the study area was chosen to follow the general line of highest groundwater elevation. The water table in the Chalk slopes generally westwards, but with local deviations corresponding to the topography of valleys and interfluvial areas.

In the two lower aquifers, unconfined conditions occur beneath the areas of their outcrop, with water table configurations related to the local topography, but again descending regionally towards the west. The eastern parts of these aquifers show confined conditions as they dip gently beneath their respective overlying aquitards. Thus, there is potential for natural or artificially induced leakage between the three aquifers, by means of flow across the intervening aquitards. In the northern half of the modelled area, the upper of the two aquitards is composed of a thin layer of Red Chalk, which has considerable permeability. Thus, in this area, there is moderately good hydraulic continuity between the Chalk and Carstone. Further south, this continuity is greatly reduced because of the development of Gault Clay. The lower aquitard, Dersingham Clay, is more continuous across the whole area.

Abstraction occurs at 160 private wells and 12 major pumping stations for public water supplies. Some pumping stations remove water from the Chalk, others from the lower aquifers. In the latter case, the reduction of heads in the lower aquifers may induce recharge by vertical leakage from the groundwater in the Chalk. Thus, for water resources purposes, a model must represent this leakage accurately. (AWG, 1997).

Recharge to the Chalk aquifer occurs from rainfall and infiltration on its outcrop, and from groundwater moving downwards through the cover of glacial deposits in the east. Average annual precipitation over the modelled area is 648 mm. River flow in the Nar averages 1.1cumecs over the catchment area with a baseflow proportion of 83 %. Although the Wensum is fed by Chalk groundwater, its proportion of baseflow is much lower, as the areas of glacial clay promote runoff and reduce infiltration. (Boar *et al.*, 1994).

Natural recharge to the lower aquifers occurs from precipitation on their outcrop areas, with minor contributions via leakage through overlying aquitards. The leakage contribution may be locally increased where abstraction from the confined zones has increased vertical hydraulic gradients.

River discharge records of varying lengths are available for each of the major rivers, and the area contains hundreds of wells at which water levels can be observed.

5. The "template" model in AQUA-3D

A model based on the finite element AQUA-3D code was developed prior to the present study by Vatnaskil Consulting Engineers and Land and Water Resource Consultants of Histon, Cambridgeshire, on behalf of Anglian Water Services plc (AWG, 1997). This model formed the starting point of the present work, and is briefly described here.

The AQUA-3D model is based upon a horizontal finite element mesh made up of 4000 triangular elements. Observation boreholes and abstracted wells were used to constrain the mesh by locating them at the apices of the elements. Rivers were modelled as lines of element edges (fig. 1). The layered structure of three superposed aquifers was represented by three layers of mesh in the model, with the aquitards being represented by vertical conductivity between them. For computing water flows, each element within each layer possesses attributes of top and bottom elevation, hydraulic conductivity, transmissivity, storativity, and vertical conductivity to the model layer above. The FE method solves groundwater heads (potentials) and flow (streamlines) within each element, while maintaining continuity of heads and flows across element boundaries. (Wang and Anderson, 1995).

The boundary conditions chosen for the model area as follows. At the northern and western boundaries, where aquifers are in contact with the sea, a contant-head condition was used. In the north, the lowest aquifer lies below sea level, and were assigned impermeable boundaries. The southern and eastern boundaries approximately coincide with groundwater divides in the Chalk, and these were represented in the model as impermeable boundaries. The outcrops of middle and upper aquifers have limits in the west which lie some distance from the edge of the FE mesh, as this was designed to include the more extensive outcrop of the lowest aquifer. Where an aquifer layer is absent in reality, the mesh elements were assigned zero thickness (effectively zero transmissivity).

Outflows from the modelled aquifers occur via groundwater flow upwards or downwards through the inter-stratified aquitards, and via discharges to rivers and springs. Springs were represented as constant heads nodes, and rivers as chains of constant head nodes. The AQUA-3D code computes groundwater seepages to rivers by treating them as a special type of areal boundary, known as a "back-and-forth" boundary. Essentially, the river is treated as a line sink, with head specified at nodal points along the length.

The model is driven by recharge, which was calculated externally to the groundwater modelling package using a proprietary surface-groundwater interaction programme developed and operated by Vatnaskil Consulting Engineers. This package was calibrated using river flows at gauging stations as a modelling target. The output consisted of baseflow and runoff components of river flow, plus infiltration from the surface model to aquifers. The surface model was calibrated against river flow values from 1988 to 1997. The infiltration output from this model consisted of 302 areal domains each with a time-series infiltration for these years. These infiltration values were used to drive the AQUA-3D groundwater model (AWG, 1997). The same values were adopted for the MODFLOW model described below.

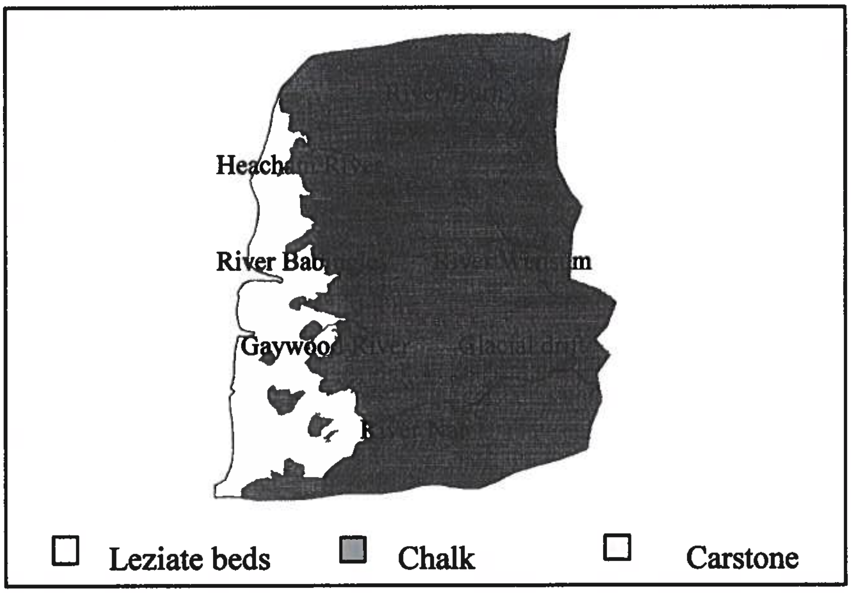

Figure 1. Model boundaries and areas of outcrop of the tree aquifers, plus glacial drift cover on the Chalk

The AQUA-3D groundwater model (AWG, 1997) was calibrated by trial-and-error adjustment of hydraulic parameters for each element, with values constrained by field measurements (e.g. from pumping tests) and by the principle that adjacent elements should as far as possible share the same values so as to make up uniform domains. The calibration targets were observed time-series of groundwater heads at 30 observation wells. The historical records of abstractions from major pumping stations were used in the model, whereas minor abstractions were approximated from data on licensed consents. The model gave satisfactory fits to the calibration records, as described in unpublished reports (AWG, 1997). Fig.4 shows the FE mesh and the calibrated hydaulic conductivity field for the layer representing the Chalk.

The files detailing the domains of parameter values plus input, output and calibration data for the AQUA-3D model were kindly supplied to the present project by Anglian Water Services plc. From these files, we were able to take the parameter values for each element, and to transfer them with as little distortion as possible to the finite difference MODFLOW model described below.

AQUA-3D model in steady state

AQUA-3D is a transient-flow FE model. To develop an equivalent FD model using MODFLOW we require a realisation of steady-state groundwater flow, because of the limitations of MODFLOW in representing transport during transient flow conditions. For this purpose, therefore, it was necessary to develop a steady-state representation of the study area, using AQUA-3D. This was accomplished by forcing the model from its calibrated 1997 finishing state, using a time-series of non-varying recharge and abstraction values which were equivalent to the average for the previous 11 years. A time step of one day was employed and fluxes entering or leaving the system and any changes in storage were computed by the model at each time step. Steady state conditions took the equivalent of 13 model years to be achieved. For the model period in which steady conditions had been achieved, leakage, pumping, infiltration, outputs or inflows from the springs and rivers, and flows across the boundaries were added up. The result represents the water balance for the system which should be very close to zero. Fig.2 shows the steady state field of groundwater heads determined by AQUA-3D in this way.

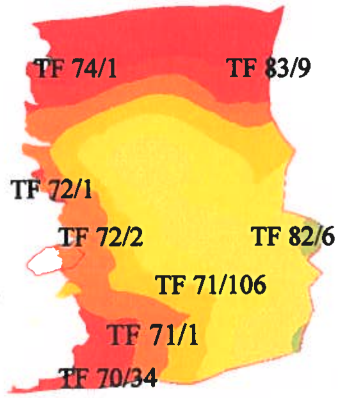

Figure 2. Groundwater heads at steady state

6. Construction of the MODFLOW model

A numerical model, based on the MODFLOW code, was developed to simulate existing groundwater flow conditions around the site. The package was developed by the United States of Geological Survey (McDonald & Harbaugh, 1988). The MODFLOW model is based upon a the finite difference (FD) mesh consisting of 80 rows and 70 columns spaced every 500meters (Fig. 3). The grid is made up of 3896 rectangular elements of 0.25km² in area. Model boundary conditions similar to those in AQUA-3D were defined along the edges of the simulation domain. Where an aquifer unit is absent, it was assigned zero transmissivity. In the north and west, constant head boundaries were used where aquifers meet the sea, with impermeable boundaries for the limits of aquifers that lie below sea level. On the southern and eastern boundaries, a no-flow condition was used. With the model domain, springs were represented by constant head nodes. Well abstractions were represented by specifying discharges equal to the sum of the abstractions from all the wells within grid cells that contained them. MODFLOW's river-cell package was used to model the major rivers and their interaction with groundwater, with bed parameters chosen to give equivalent hydraulic behaviour to the aquifer beneath the river in each cell.

The relationship between the three aquifers was modelled by MODFLOW in a similar way to AQUA-3D, by means of three layers of cells representing the aquifers, and leakage conductances between them to represent the aquitards. However, an extra layer was added above the Chalk to simulate the surface features. Specifying the properties of this layer created a dilemma. In areas where the Chalk is close to the ground surface, the real aquifer is unconfined. Here the extra layer could be made very thin, with the same properties as the cell beneath. Where the Chalk is drift-covered, it is also in many places confined, because in reality recharge occurs by downward groundwater flow through the drift. Yussolf et al (2002) modelled the drift layer explicitly in a MODFLOW representation of the Chalk aquifer to the south of our study. Leakage to the underlying Chalk was determined in their model by adjusting the vertical hydraulic conductivity to the boulder clay layer, while maintaining its heads at elevations close to the ground surface. This model formulation could not be used in the present study, because recharge values were taken from AQUA-3D, for which they were determined through a separate runoff model, as described above. Thus, the recharge values driving our MODFLOW model already embodied the hydrological effects of the glacial drift cover. Therefore it was not appropiate to give the new layer in our model the actual properties of the drift. Instead it was given hydraulic properties equivalent to the underlying Chalk. The main function of this layer in our model was thus to determine where confined conditions would occur in the Chalk layer, and to prevent the model from simulating the overflow of groundwater to the surface in such places. The four layers of the MODFLOW model were numbered from top to bottom as follows: Drift (model layer 1), Chalk (model layer 2), Carstone (model layer 3) and Leziate Beds (model layer 4).

The simulation domain is subdivided into a number of zones having different hydrologic properties. Property values were transferred manually from the AQUA-3D model by overlaying the FE mesh with the MODFLOW grid. Fig. 5 shows the field of hydraulic conductivity for the Chalk as an example.

Recharge was represented on the uppermost MODFLOW layer by transferring the infiltration values from 302 zones on AQUA-3D model onto corresponding cells in the FD grid. The annual infiltration values for each zone were added up and divided by the length of the record, 13 years., to give an average value for each zone which was then expressed in terms of metre depth of water per second.

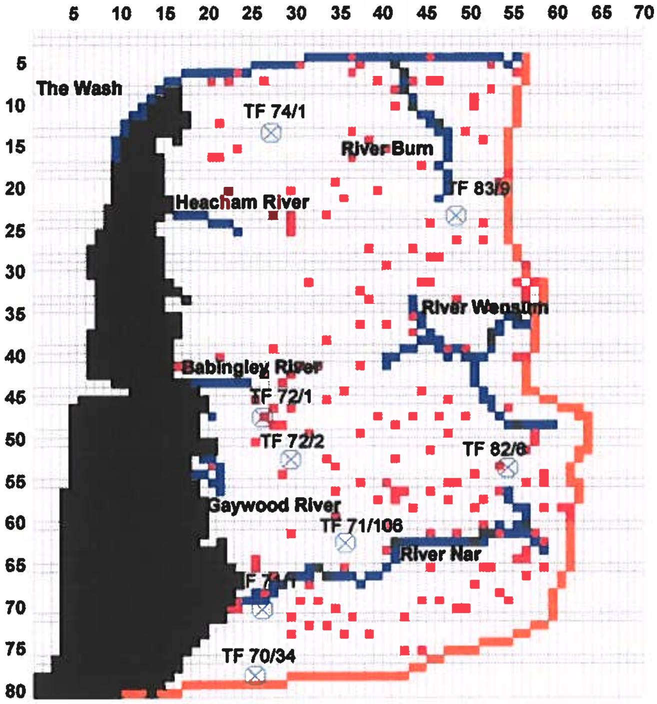

Figure 3. FD mesh. Regional Flow model in MODFLOW

MODFLOW model results at steady state

Once the model had been built, the MODFLOW solver was run to generate and display head contour lines and flow vectors at steady-state. This gave an initial estimation of groundwater flow regime within the model.

Fluxes were estimated through analysis of the results from the MODFLOW model run at steady state. Because the parameter values of MODFLOW were set as close as possible to those in AQUA-3D, there was no need to make large adjusments in any of the hydraulic parameters. The general patterns of flow in the two models were very similar.Remaining discrepancies can be attibuted to the different structures and formulation of the models. To eliminate these, small adjustments were made to hydraulic conductivity. Recharge can be altered, and a small discrepancy does arise because of the errors in tranferring from a triangular mesh to a grid. Other parameters were not altered.

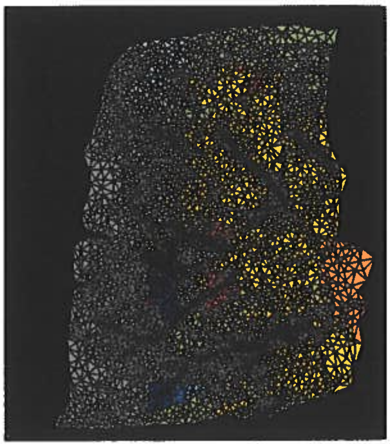

Figure 4. FE mesh. Hydraulic conductivity field for layer 1 (Chalk) in AQUA-3D.

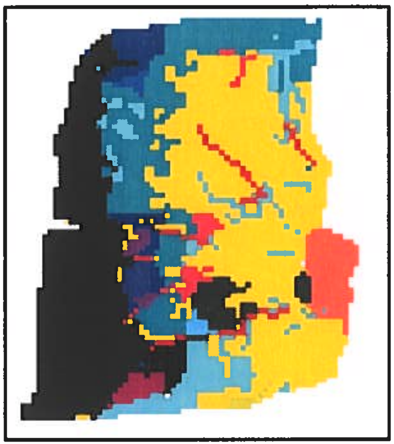

Figure 5. Hydraulic Conductivity: Areal Parameter representation for Layer 2 (Chalk) in MODFLOW

7. Results

As described in the previous section, our major interest for risk assessment is in the Chalk for which water balance was estimated.

Table 2 summarizes the volumetric budget for both models at a steady state, the finite element model (FE) using AQUA-3D and the finite difference model (FD) using MODFLOW.

	AQUA-3D		MODFLOW	
Contribution of:	**IN**	**OUT**	**IN**	**OUT**
Pumping		-0.50		-0.50
Leakage	2.50		2.87	
Storage		-0.03		
Infiltration	2.32		2.29	
Boundary Conditions		-4.29		-4.52
TOTAL	4.82	-4.82	5.16	-5.02
IN – OUT (m^3/sec)		0.00		-0.14
Error (%)		0.00		2.71%

Table 2. Water Balance

Recharge occurring on the uppermost layer and the leakage between the Drift and the Chalk represent the main inflows to the system; balancing these abstraction through pumped wells and discharge to rivers contribute to the outflow. The total influx of water in the AQUA-3D model is 4.82 cumecs and using MODFLOW is 5.16cumecs, whilst corresponding outflows are 4.82 cumecs in AQUA-3D and 5.02 in MODFLOW respectively. The discrepancy of 6.59% in inflows and 3.98% in outflows seen between the two models results rely mainly from the gridding used by the two models. In the FD model, the rectangular cells ignore those smaller areas in which recharge is reduced to zero. A small adjustment has been made to correct this and reduce the initial recharge difference.

The calibration results were assessed using the differences between calculated heads at eight targets sites. These targets were distributed fairly uniformly through the domain; that is, their locations were not clustered in a single area but rather near the different flow boundaries previously defined. Six of the targets (TF72/1, TF2/2, TF83/9, TF82/6, TF71/106, and TF1/1) were located near to rivers. They made major contributions to the total flow through the models observing change in flow direction. A seventh target (TF74/1) was placed near the constant head boundary, where the aquifer is close to the sea. The last target (TF70/134) was placed near the impermeable boundary in the south. (Fig. 3)

In table 3, a comparison of differences observed in water levels at those eight points provides a basis to evaluate the accuracy of the model.

Target	AQUA-3D (m)	MODFLOW (m)
TF 70/34	13.08	10
TF 71/1	11.36	10
TF 71/106	26.83	25
TF 72/1	23.75	20
TF 72/2	30.49	30
TF 74/1	4.33	5
TF 82/6	54.65	50
TF 83/9	20.87	20

Table 3. Groundwater Heads at Steady State

An important calibration criterion was flow direction since this could be estimated fairly accurately from Chalk aquifer data. In both models, the flow vectors point to no-flow boundary in the east, toward the North sea in the north and also their direction converges to the river flow line.

8. Conclusions

Model construction has been a time consuming task in this project due to the large number of cells and the need to apply flow boundaries and hydraulic properties to each one separately.

A fundamental discrepancy between the two models is introduced by the transferring of hydraulic parameters from triangular elements to rectangular cells. However, the evaluation of the nature and the magnitude of differences calculated for fluxes at steady state confirm that the two models match well.

The approach used in this work demonstrates that a good match of the two models has been achieved after aquifer responses from the FE model (such as flow and head fields) were compared to corresponding values obtained from the FD model.

Acknowledgements

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References

AWG, Groundwater modelling of the Chalk and Sandringham Sands aquifers of North West Norfolk, Cambridgeshire, 1997.

BGS, Geology of the country around King's Lynn and the Wash, British Geological Survey, London, 1994, p. 100-136.

Boar, R.R, Lister, D.H, Hiscock, K.M & Green, F.M.L., The effects of water resources management on the Rivers Bure, Wensum and Nar in North Norfolk, July 1994, National River Authority.

Funnell B. M., Larwood G.P., *The geology of Norfolk*, London, 1970.

Hiscock, K.M., *The hydrogeology of the Chalk aquifer system of North Norfolk*, Bulletin of the Geological Society of Norfolk, no. 41, 1991, p. 3-43.

Hiscock, K.M, Lister, D.H, Boar, R.R & Green, F.M., *An integrated assessment of long term changes in the hydrology of three low lands rivers in Eastern England*, Journal of Environmental Management, no.61, 2001.

Hydrological Survey, *River Great Ouse Basin: Hydrometric Area no. 33*, Ministry of Local Government, London, 1960.

Hydrometric Register and Statistics 1986-1990: A catalogue of river flow gauging station and observation boreholes with summary hydrometric statistics, London, 1993.

Hydrological Map of northern East Anglia 1:125000, Institute of Geological Sciences, London, 1976, Institute of Geological Sciences.

Larwood G.P., B.M. Funnell, *The Geology of Norfolk*, Headley Brothers Ltd., London, 1970. Groundwater modelling of the Chalk and Sandrigham sands aquifers of North West Norfolk, Cambridgeshire, 1997, Anglian Water(AWG).

Lloyd, J.W., The United Kingdom. In: Downing, R.A., Price, M., Jones, G.P., The Hydrogeology of the Chalk of Northern West Europe, Oxford Univ. Press, 1993, p. 220-249.

MacDonald A., Allen D., *Aquifer properties of the Chalk of England*, Quarterly Journal of Engineering Geology and Hydrogeology, no. 34. 2001, p. 371-384.

Ming-Hsu Li, Hwai-Ping Cheng, *Solving 3D Subsurface Flow and Transport with Adaptive Multigrid*. Journal of Hydrologic Engineering, 2000, p. 74-80.

Surface water United Kingdom 1977-1980: A register of United Kingdom gauging stations with selected hydrometric statistics, catchment rainfalls and river water temperatures.

Yussoff I., PhD thesis, 2000, University of East Anglia.

Wang, H.F., Anderson, M.P. *Introduction to Groundwater Modelling*. Finite Difference and Finite Element Methods, 1995, San Francisco (USA), Academic Press Inc.