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REPRESENTATION OF THE VARIATION OF HYDRAULIC CONDUCTIVITY WITH SATURATED THICKNESS IN MODFLOW

STAGES I & II. CODE CHANGES AND TESTING AGAINST BIRMINGHAM UNIVERSITY CODE

TECHNICAL NOTE

National Groundwater & Contaminated Land Centre Project NC/99/67

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TECHNICAL NOTE

Introduction

This technical note presents a summary of work carried out to improve the representation of groundwater flow processes in chalk and limestone aquifers managed by the Environment Agency. It is standard practice to evaluate groundwater resources using numerical models, which simulate the response of the heads and flows in an aquifer to abstraction, recharge and surface water interactions.

The Agency has decided to adopt MODFLOW (McDonald & Harbaugh 1988, and 1996) as a "best interim solution" for in-house groundwater flow modelling. It is an industry standard code that has been rigorously tested and evaluated; it simulates river/groundwater interactions, and is compatible with particle tracking codes. The Agency is keen to develop improvements to MODFLOW where it's capabilities fall short of those needed to accurately model the flow behaviour of British aquifers. This is intended to provide a more reliable basis for resource assessment and management. As part of this work, a project was commissioned to include a mechanism to allow horizontal hydraulic conductivity to vary with depth in MODFLOW. Full implementation of this mechanism is being carried out in stages. This overview summarises the work carried out in Stages I and II.

Objectives and outputs

The Environment Agency is continually improving its understanding of groundwater systems in the UK. Knowledge of these systems often exceeds the capabilities of the modelling tools that are used to represent them. The aim of the current project is to help bridge the gap between what is known about chalk and limestone aquifers, and how this knowledge can be represented within a numerical model in order to improve resource evaluation and hydrological impact assessment.

The objectives of the project can be summarised as follows:

- To incorporate the relationship between hydraulic conductivity and saturated depth used in the University of Birmingham code (Figure 1) into MODFLOW, and to test it against the Birmingham code.
- To investigate the strengths and weaknesses of MODFLOW when large-scale code changes are undertaken.
- To make an initial assessment of how well MODFLOW's stream package is able to represent ephemeral streams.

The output of the project consists of a new operational version of MODFLOW, a user manual and a project report. The changes to the MODFLOW code have been made in such a way as to make the new version backward compatible. This means that the modified code can be used with MODFLOW '96 data files.

Background

Modelling groundwater flow in chalk and limestone aquifers is one of the more demanding problems encountered within the context of British hydrogeology. These aquifers are typically highly permeable, low storage systems in which the heads and flows respond extremely quickly to recharge. Relatively acidic recharge causes solutional enlargement of fissures where groundwater flow predominantly occurs. This results in variations in hydraulic conductivity, generally with values increasing towards river valleys and decreasing with depth. The higher hydraulic conductivity near the water table often results in a good hydraulic connection with surface water; spring discharge can be extremely high (hundreds of Megalitres per day). Discharge is closely related to groundwater head, which in turn is related to hydraulic conductivity. Changes in groundwater levels can result in the head of streams moving several kilometres seasonally, resulting in ephemeral stream flow. It is important to model these features because improved representation of processes is considered to result in improved resource evaluation.

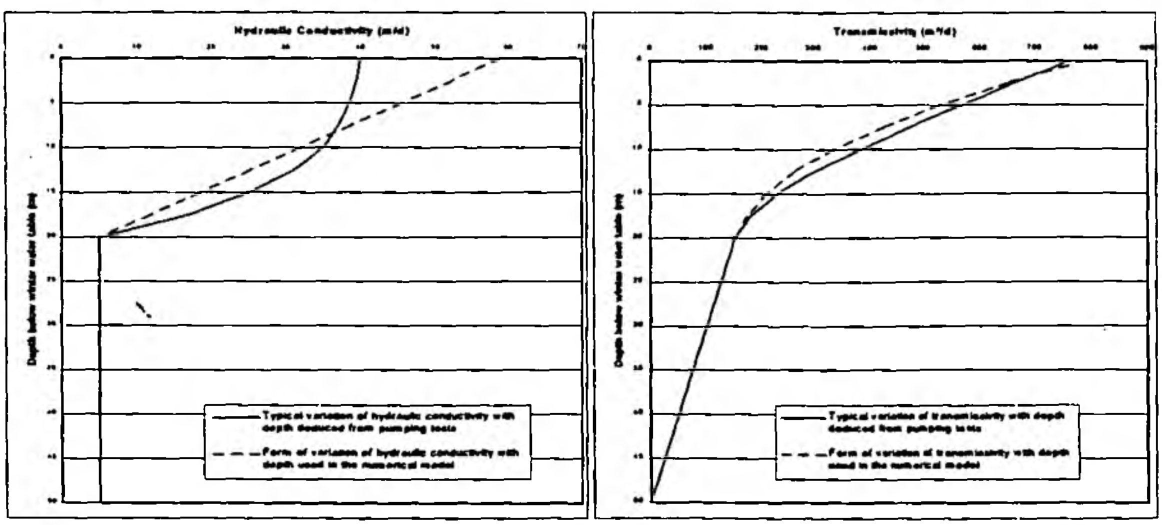
The issues associated with modelling chalk and limestone aquifers that have been addressed in this project are summarised below.

Variation in horizontal hydraulic conductivity with depth (VKD)

The representation of variation in hydraulic conductivity with depth in groundwater flow models has traditionally required the specification of multiple model layers. When predicted water level fluctuations exceed layer thickness, layers can become 'dry' and numerical difficulties can occur during 're-wetting'. Allowing variation in hydraulic conductivity with depth in a single layer offers significant potential computational advantages.

The importance of including variable hydraulic conductivity with depth in groundwater models was identified during a study of pumping tests in the Berkshire Downs (Rushton & Chan 1976). The same borehole was tested at two different times. In the first test, when the rest water level was high, a large yield was maintained for 14 days but in the second test when the rest water level was 7.5 m lower excessive drawdowns occurred after only five days with a lower pumping rate. Subsequent analysis confirmed that the responses could only be produced by an increase in hydraulic conductivity in the zone of seasonal water table fluctuation. This was an essential feature incorporated in a regional groundwater model of the Berkshire Downs, which was constructed at The University of Birmingham (Rushton, Connorton & Tomlinson, 1989). In the valleys the zone of water table fluctuation is only a few metres but the hydraulic conductivity and its rate of change with depth is high. In the interfluves it is the reverse; the zone of fluctuation may be tens of metres but the hydraulic conductivity and its rate of change with depth is low.

Figure 1 Conceptual diagram of the relationship between hydraulic conductivity and depth



A typical distribution of hydraulic conductivity with depth in the chalk, and how this is represented in the Birmingham University model ("The Birmingham Code") is presented in Figure 1 (after Rushton et al, 1989). The field data required to define the variation of hydraulic conductivity with depth can be obtained by repeating pumping tests at different times of year with different initial water levels, or from packer tests, geophysics or a comparison of groundwater levels with river flows. In addition to improving estimates of the groundwater resources of the Berkshire Downs, this approach has proved crucial in models of other chalk and limestone aquifers including those found in South Humberside, Yorkshire, Lincolnshire and East Kent.

Variation in storage with depth

In chalk and limestone aquifers, the drainable proportion of matrix material is usually very small (<1%). Specific yield is controlled by drainage of the fissure system; its value being dependent on the extent of fissure development. Typically, solution enhancement of fissures decreases with depth so that, as the water table falls, unconfined storage will also decrease. This has been identified as an important mechanism affecting groundwater behaviour in the Candover catchment (Rushton and Rathod, 1980).

Surface water features

Surface water features play an important role in providing flows to or from an aquifer. It is important to understand how interaction occurs with the groundwater system. Springflow and ephemeral streams are key mechanisms by which water leaves a chalk or limestone aquifer system. Rivers and streams also form a significant component of recharge and hence resources when groundwater levels are depressed in relation to river levels.

Starting conditions

Experience of modelling these complex, non-linear systems has revealed a need for care when producing the starting conditions for time-variant simulations, in order to avoid numerical instabilities. In particular, work carried out at The University of Birmingham has shown that stable starting conditions are best produced by initially using a simplified model with specified transmissivities to calculate a head distribution.. The complexity of the head dependent transmissivity calculations is introduced once this initial solution has been obtained. Work was required under this project to include this procedure in the MODFLOW code.

Modifications to the MODFLOW code

The following mechanisms have been investigated and incorporated into MODFLOW as part of this project:

- Variation of horizontal hydraulic conductivity with depth (VKD): a linear increase in hydraulic conductivity is permitted within the zone of water table fluctuation

- Variation of storage with depth: a sharp change from one storage value to another is permitted at the bottom of the zone of fluctuation

- The existing MODFLOW stream package has been tested in conjunction with VKD. The code was modified to allow an abstraction or inflow to be specified at any point along a stream reach.

Other features that have been added to MODFLOW during this project include:

- Spatially varying anisotropy (based on method by Kladias & Ruskauff, 1996) – changing layer anisotropy to cell-by-cell anisotropy to allow T_X and T_Y values (or T_X:T_Y ratio) to be specified at each cell.
- Inter-nodal transmissivities – MODFLOW is block-centred and so had to be adapted so that a direct comparison could be made with the node-centred Birmingham code.
- Automatic calculation of VKD parameters during the calculation of starting conditions using a simplified steady state model.
- Output of the calculated inter-nodal transmissivities to the listing file.

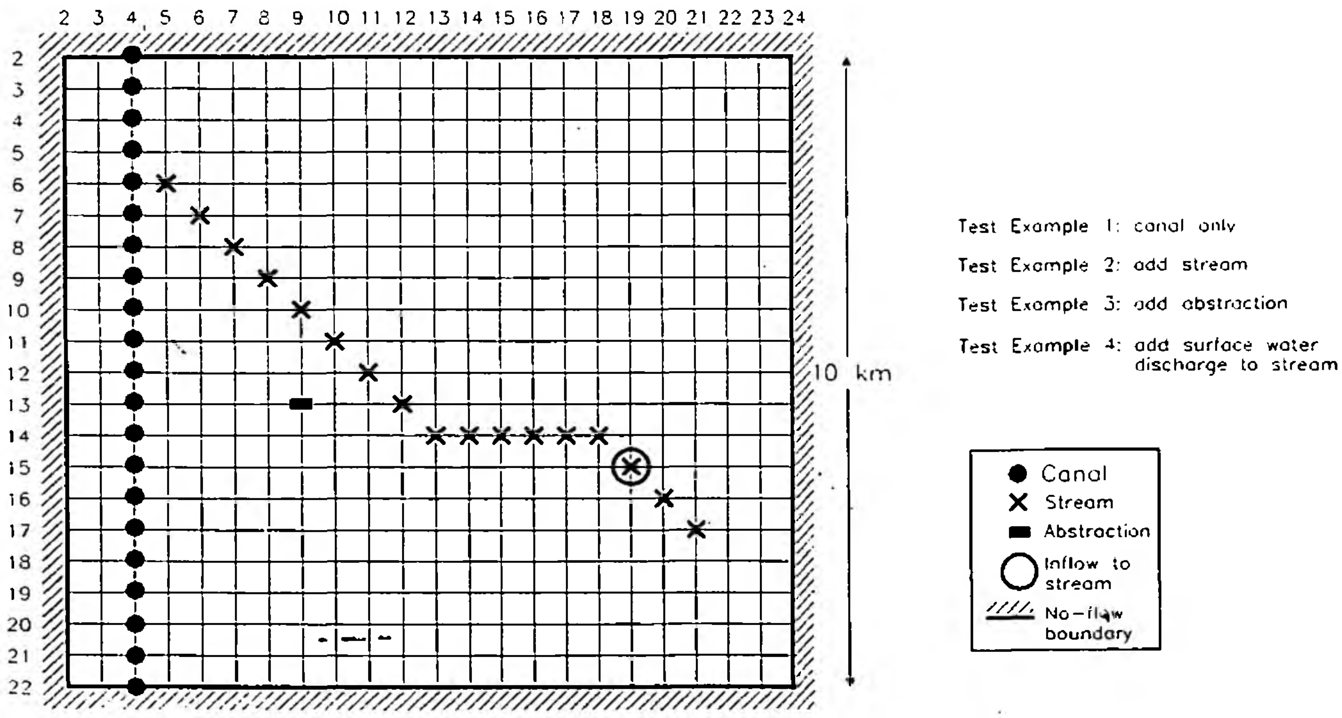
Test Examples

The modified version of MODFLOW was tested against the Birmingham code using test examples in order to provide convincing evidence that the process has been undertaken successfully. A sequence of four test models was developed using the Birmingham code. The testing programme was split into two stages; the first being to test the implementation of the variable hydraulic conductivity with depth (VKD) mechanism itself and the second stage involved further testing of VKD in conjunction with an ephemeral stream. The four test examples were developed in the following sequence, each step representing an increase in system complexity (Figure 2):

- Test Example 1: seasonal recharge and outflow to a canal,
- Test Example 2: addition of an ephemeral stream,
- Test Example 3: addition of a groundwater abstraction well,
- Test Example 4: addition of an inflow to the upper reaches of the stream (eg, from a sewage treatment works discharge).

A number of acceptance criteria were specified to determine how well the modified MODFLOW code could reproduce the Birmingham model results. These criteria included comparisons of the water balance, the groundwater heads and flow accretion along the ephemeral stream.

Figure 2 Test Example model layout



Results

Modifying MODFLOW

MODFLOW has a modular structure and the code is generally well laid out and documented. New packages can be added easily, but changes to the code require care. This is mainly due to the widespread use of conditional statements in conjunction with GOTO statements. The main areas of the code that were investigated during this work include:

- The structure of the code and the overall algorithm.
- The calculation of transmissivity based on VKD.
- The numerical solvers.
- The stream flow package.

Additional insights into the behaviour of MODFLOW have been gained from this investigation including:

- The water balance errors at every cell are not always within the maximum residual flow criterion as specified in the PCG (Preconditioned Conjugate-Gradient) solver package. This means that water balance errors should be checked independently (eg, using ZONEBUDGET (Harbaugh, 1990)) following the completion of a simulation.
- Although the PCG solver was used for most of the simulations, the SIP (Strongly Implicit Procedure) solver was also used, both solvers provide acceptable solutions to VKD problems.

All new components of the modified code were tested in a variety of steady state and time variant simulations in conjunction with different MODFLOW options and numerical solvers. All these components performed well and are compatible with the original features of the code.

Variable hydraulic conductivity with depth

The VKD mechanism was tested against the Birmingham code using all the test examples. Most of the acceptance criteria were met for the duration of all the test example simulations. The water balance errors at each node were less than 0.5%; calculated transmissivities were within 1% of those calculated by the Birmingham code, and calculated heads and global water balance were within 0.5% of those from the Birmingham code. The few occasions where the criteria were narrowly missed were found to be due to minor problems in the Birmingham code (fluctuations were caused by resetting stream length every time step, and convergence issues with stream nodes becoming inactive).

Initial conditions

The initial conditions for a time variant simulation using the VKD mechanism can be obtained in three steps, now automated within the code. The first step runs a steady state model with fixed transmissivities, the results of this simulation are used to calculate the VKD parameters in step two. The third step is to run a second steady state model with VKD active, using the parameters calculated in step two, and using the head distribution calculated in step one as the initial conditions. This reduces the chances of instability and helps avoid the problems associated with using inappropriate starting conditions.

Ephemeral streams

The only change made to the MODFLOW stream package was to allow an inflow to be added to any stream flow node. Rather the investigation focussed on comparison of results with those from the Birmingham code. Testing has confirmed that the stream package is a reliable tool for modelling surface water – groundwater interactions. Simulations using this package were found to be more stable than the equivalent simulation using the Birmingham code. The package also includes an option to calculate the stream stage, which is a feature not supported by the Birmingham code. The differences between the accreted flows calculated by MODFLOW and the Birmingham code were well within the 2% acceptance criteria specified for the test examples.

Conclusions

The output of this project is a fully functioning, backward compatible version of MODFLOW which allows for vertical variation of horizontal hydraulic conductivity in the upper layer of a groundwater flow model. The code has been tested against code developed at the University of Birmingham and the results show that the new version of MODFLOW performs as well if not better than the Birmingham code. Specific findings of the work carried out in Stages I and II are:

- The modified MODFLOW code provides an accurate way of representing the variation of hydraulic conductivity with depth without the need to specify multiple layers in a model.
- The VKD mechanism offers an improvement over the constant hydraulic conductivity option when modelling outflows to rivers, the modelled river flows are much more realistic (ie higher in winter and lower in summer). This is a significant advantage when modelling the highly variable flows that are observed in the rivers and streams located on chalk and limestone aquifers.
- The initial conditions for a VKD simulation can be obtained by running a specified transmissivity simulation prior to the VKD simulation. This is undertaken automatically in the modified code.
- The MODFLOW stream package can represent an ephemeral stream as successfully as the Birmingham code.
- Insights into the behaviour of the PCG solver in MODFLOW were gained concerning water balance errors.

Overall, the work has suggested that it is more effective to adapt a code to include the mechanisms observed in the field than to constrain the conceptual model to include only the mechanisms available in the code.

Future work

This project was originally conceived as being undertaken in three stages. Progress at the end of Stage II is encouraging. The modified version of MODFLOW has now been tested using some example problems; the main test of the code will be its success in modelling a real system on a regional scale. Work in Stage III will focus on an investigation of the modified code using the existing South West Chilterns MODFLOW model. Further work will be undertaken on the Itchen and other models currently under development by the Agency. Additional potential improvements are listed below:

- The VKD mechanism will be developed for use with multi-layer systems so that it can model either unconfined or convertible layers and be located below other layers.
- The VKD mechanism can be tested with further features of ephemeral streams, eg multiple streams, to investigate the following: the effect of a moving groundwater divide; stream – aquifer interaction over a confined / unconfined boundary; leakage creating a dry section in the middle of a stream reach.

The following have been identified as possible directions for future work to improve MODFLOW:

- The variation of storage with depth (VSD) could be refined to allow a gradual increase of storage with water table elevation
- Improvements to the calculation of vertical flows: making use of variations in saturated thickness and vertical hydraulic conductivity.
- Improvements to the well package to allow an estimate of dynamic head in the well and the control of well rates according to this head
- Head dependent mechanisms to represent groundwater outflow to wetlands
- Alternative methods for representing "dry" cells

As aquifers become more fully exploited, the availability of groundwater resources increasingly scarce and impacts increasingly felt, it is in the interests of the Environment Agency that a programme of assessing and improving modelling software and its application to aquifers managed by the Agency should be continued.

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