EA-NGWCLC

ENHANCEMENTS TO MODFLOW

VARIATIONS IN HYDRAULIC CONDUCTIVITY AND STORAGE WITH DEPTH

National Groundwater & Contaminated Land Centre Project NC/00/23

ENHANCEMENTS TO MODFLOW

VARIATIONS IN HYDRAULIC CONDUCTIVITY AND STORAGE WITH DEPTH

National Groundwater & Contaminated Land Centre Project NC/00/23

Research Contractor:
Water Management Consultants Ltd
23 Swan Hill
SHREWSBURY SY1 1NN

Environment Agency
National Groundwater & Contaminated Land Centre
Olton Court
10 Warwick Road
Olton
Solihull B92 7HX

National Groundwater & Contaminated Land Centre Project NC/00/23

Publishing Organisation:
Environment Agency
Rio House
Waterside Drive
Aztec West
Almondsbury
Bristol BS12 4UD
Tel: 01454 624400 Fax: 01454 624409

ISBN: 1 857 05765 1

Dissemination status
Internal: Released to Regions
External: Released to Public Domain

Statement of use
This report documents the work carried out in modifying the MODFLOW groundwater modelling code to include a method for representing the variation of hydraulic conductivity with depth. The method used is based on that included in the model code developed by the school of Civil Engineering at the University of Birmingham. The information within this document is for use by Environment Agency staff and others involved in water resources management and groundwater modelling. This work is a continuation of that begun in 1999

Research contractor
This document was produced under a National Groundwater & Contaminated Land Centre Project by:

Water Management Consultants Ltd
23 Swan Hill
Shrewsbury
Shropshire
SY1 1NN
Tel: 01743 231793 Fax: 01743 232894

Environment Agency's Project Manager
The Environment Agency's Project Manager for this project was:
Paul Hulme
The Project Board consisted of:
Paul Hulme, Paul Shaw, Andrew Longley, David Johnson

National Groundwater & Contaminated Land Centre Project NC/00/23

ENHANCEMENTS TO MODFLOW

VARIATIONS IN HYDRAULIC CONDUCTIVITY AND STORAGE WITH DEPTH

March 2002

1621/R1

Prepared for:

National Groundwater and Contaminated Land Centre
Environment Agency
Olton Court
10 Warwick Road
Olton
Solihull B92 7HX
UK

Prepared by:

Water Management Consultants Ltd
23 Swan Hill
Shrewsbury
Shropshire SY1 1NN
UK

CONTENTS

TECHNICAL NOTE

The work presented in this report forms part of the Environment Agency's continuing work to make enhancements to the groundwater modelling code MODFLOW (McDonald & Harbaugh, 1988; Harbaugh & McDonald, 1996), so that it includes features that are important in UK hydrogeology. The first of these enhancements was to include a variation of hydraulic conductivity with depth (VKD), as is often observed in chalk and limestone aquifers. This work commenced in 1999 and is described in detail in previous project reports (Environment Agency, 1999 and Environment Agency, 2000). The work has now been extended to allow variations in both hydraulic conductivity and specific yield with depth within any model layer. Additional modifications have also been made to include extra options for the stream package (Prudic, 1989), the PCG2 solver package (Hill, 1990), and the MODFLOW utilities package.

Observations of groundwater behaviour in fractured systems, such as chalk and limestone formations, reveal significant reductions in hydraulic properties with depth, due to reduced fissure frequency. These fissures can also provide a good hydraulic connection between the aquifer and surface water, with ephemeral streams and swallow holes a common feature of these catchments. The variations in hydraulic properties with depth give rise to distinctive behaviour, such as large flow fluctuations in groundwater-fed streams (including ephemeral streams), different responses to pumping depending on the rest water level, and abrupt changes in water table elevations during drought.

Traditionally, chalk and limestone aquifers have been represented in groundwater models as a thin layer representing only the 'active flow zone', which is usually assumed to be between 30 and 60 m thick, with no variation of hydraulic conductivity with depth. These constant hydraulic conductivity models give rise to a linear variation of transmissivity with depth, which is a poor approximation to the observed transmissivity variation. The limited representation of the conditions in the aquifer means that, in order to represent observed behaviour the modeller may need to employ unrealistic or contrived values for other model parameters such as storage, river conductance, or temporal distribution of recharge.

An additional problem with these types of MODFLOW models is that if a severe drought is being simulated, groundwater heads can fall below the normal active flow zone, resulting in cells becoming 'dry', and distorting the pattern of flow. If a low hydraulic conductivity layer is added below the active flow zone to enable 'wetting' of the layer above, the contrast in hydraulic conductivity between the two layers often results in numerical oscillations as cells change between wet and dry, reducing the likelihood that the model will converge.

The solution to these problems is to allow hydraulic properties to vary with depth within a single model layer. This gives a non-linear relationship between transmissivity and groundwater level, improving the representation of field conditions. This kind of relationship was first included in groundwater models of the chalk constructed at the University of Birmingham, including models of East Kent (Cross et al, 1995), the Berkshire Downs (Rushton et al, 1989), Candover (Rushton & Rathod, 1980), and Lincolnshire (Rushton et al, 1982).

As part of the Agency's programme of enhancements to MODFLOW, the model code was modified to allow hydraulic properties to vary with depth within any individual model layer. The enhancements to MODFLOW were originally based on the model developed at the University of Birmingham (Environment Agency, 1999).

The original investigations showed that including a variation in hydraulic conductivity with depth results in changes in the behaviour of the groundwater models. Stream flows become more variable, and groundwater levels become less variable under normal conditions, but fall dramatically when levels fall below the normal zone of water table fluctuation. Although the variation in heads is reduced, the variation in transmissivity is increased due to the shape of the hydraulic conductivity profile. It is this profile that enables the VKD model to reproduce large variations in flow, whilst reducing the variation in groundwater heads (Environment Agency, 2000).

The enhancements to MODFLOW have now been extended to include the following additional features:

- Variations in hydraulic conductivity with depth (VKD) allowed in any layer.
- Variations in specific yield with depth (VSD) allowed in any layer.
- The auto-conversion option for converting standard MODFLOW models to VKD models has been updated to allow for multiple VKD layers and to allow the starting model to have either specified hydraulic conductivities or transmissivities.
- Allow a maximum hydraulic conductivity and/or specific yield to be specified for each model cell.
- Make changes to the stream routing package to allow discharges, abstractions or tributary inflows to be specified at any stream node.
- Include an output of model progress to the screen when using the PCG solver package.
- Allow binary output files to be in the same format as those required by Groundwater Vistas (GV – Environmental Simulations Inc, 2001), the Agency's preferred MODFLOW user interface.
- Include an option to allow the input of X- and Y-direction transmissivities or hydraulic conductivities independently (without using the anisotropy ratio method).
- Include the option to allow convergence to be forced if the convergence criteria are met for a specified number of outer iterations (this was not thought to be a particularly useful option, but was included to make the code compatible with models produced by GV).
- Allow a debugging option for the PCG solver so that the evolution of head values at each iteration could be examined – to identify problem areas in models that do not converge.

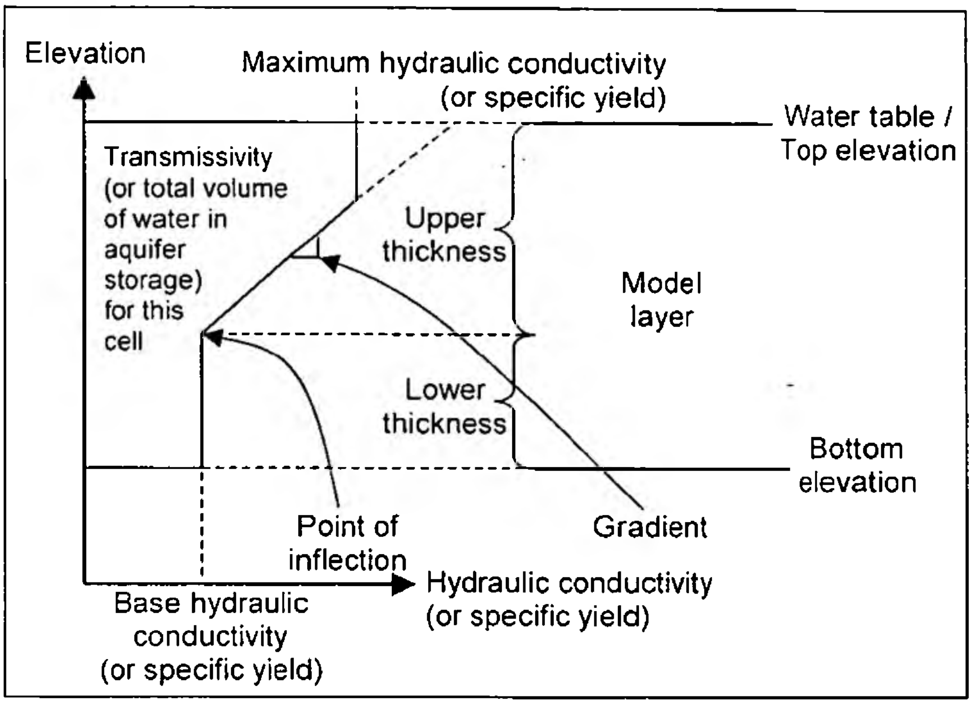


Figure 1 General form of the variation hydraulic conductivity and specific yield with depth

Figure 1 shows the general form of the profile of hydraulic conductivity and specific yield that can now be specified within any individual model layer using MODFLOW-VKD. Figure 2 gives an example of the type of situation that can be modelled using the new code.

These additional modifications have been tested using further test models, along with a regional model of the Southwest Chilterns (Environment Agency, 2000), and the Upper Lee and Itchen modelling studies (in progress). These investigations highlighted any problems with the code during its development, and ensured that the modifications worked properly. In addition, they provided insight into different practical approaches to regional scale modelling of chalk aquifers, particularly in relation to parameterisation of VKD parameters and initial conditions for time variant simulations. Insights gained include:

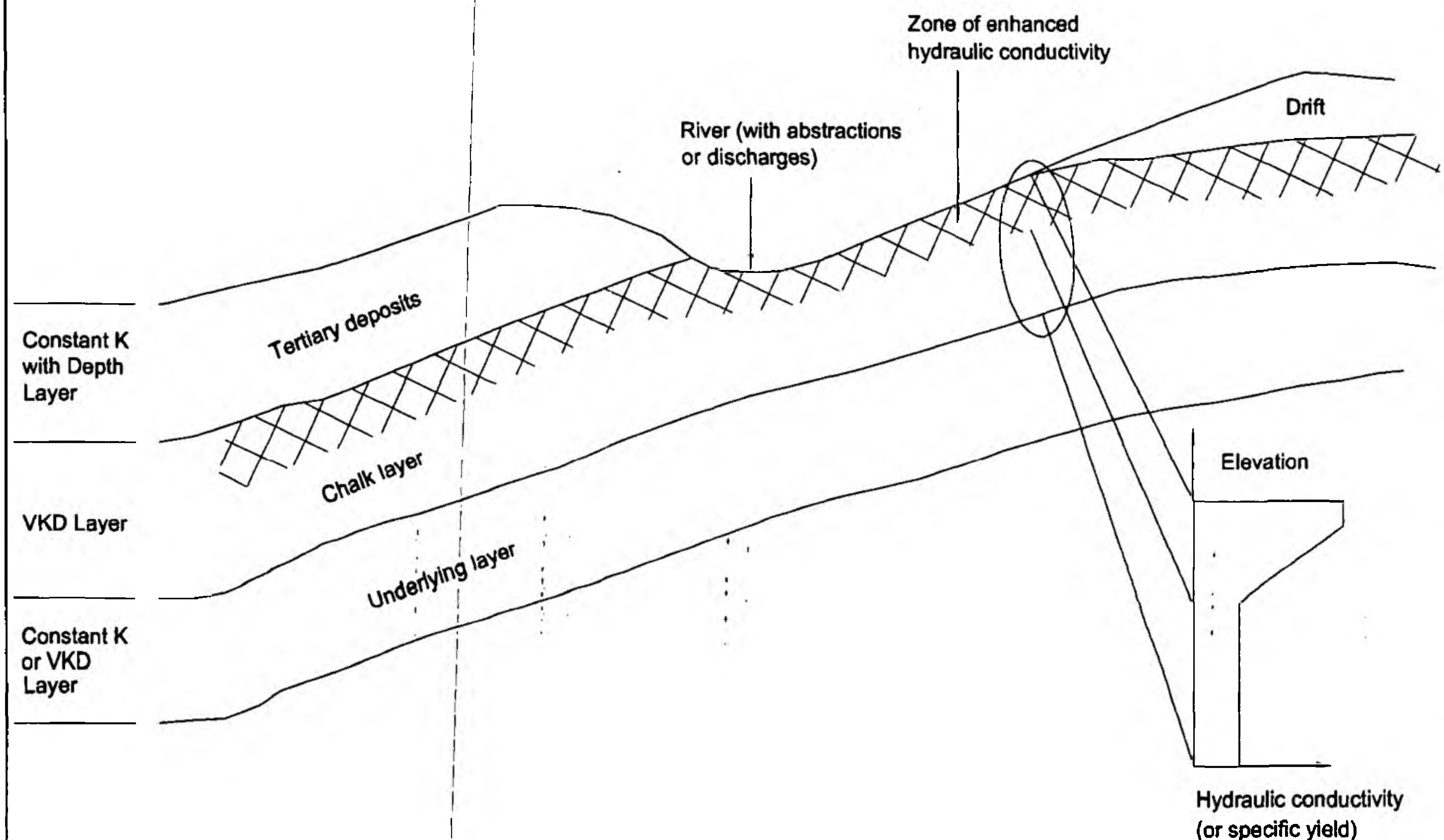
- Many different VKD profiles can give rise to the same steady state solution; differences in model results only become apparent during time variant simulations.
- In order to order to differentiate between the effects of different VKD profiles one of two approaches is required:
    - Move directly to a time variant simulation where the responses to seasonal recharge can be evaluated once the model reaches dynamic balance.
    - Conduct two steady state simulations representing the flow system under both high (spring) and low (autumn) water table conditions, in order to find a VKD profile that satisfies both these situations.
    - (The pros and cons of these two approaches are discussed in the report.)

- Approaches to avoid problems caused by 'dry' cells, especially in multi-layer models.
- Specifying a variation of specific yield with depth (VSD) often leads to instabilities (due to a necessary approximation in the code), and can result in the model not converging on a solution. Methods to avoid such instabilities are suggested, but it is recommended that this capability be avoided unless the field evidence reveals it to be an important feature of the groundwater system.
- Zoning of the hydraulic conductivity values calculated in the automatic conversion routine can make the model inputs easier to edit without drastically changing the calculated head distribution.

The changes made to the MODFLOW code allow a better numerical representation of the flow processes observed in chalk and limestone aquifers. Although the code has been developed specifically to represent chalk and limestone aquifers, it is recognised that it could also be used to model other groundwater systems where parameters vary with depth. Such applications may include:

- Any other fractured media where the fracture frequency decreases with depth (providing that the model is on a large enough scale that the fractures can be represented by an 'equivalent porous medium')
- Porous media where overburden reduces hydraulic conductivity at depth
- Systems where the hydraulic conductivity is reduced at depth due to changes in geology (providing the layers are in good hydraulic continuity and vertical head gradients are negligible)

The Environment Agency and its consultants plan further use of the modified MODFLOW code to construct groundwater models in the following areas in England: Upper Colne, N Kent, River Bourne, Ely Ouse, Kennet.



WATER MANAGEMENT CONSULTANTS

Figure 2 Typical geological setting for application of MODFLOW-VKD

1 INTRODUCTION

1.1 Background

The work presented in this report forms part of the Environment Agency's continuing work to make enhancements to the groundwater modelling code MODFLOW (McDonald & Harbaugh, 1988; Harbaugh & McDonald, 1996), to include features that are important in UK hydrogeology. The enhancements have been made in a series of stages. The first two stages of the project (Environment Agency, 1999) involved making changes to the code to include a variation of hydraulic conductivity with depth (VKD), as is often observed in chalk and limestone aquifers. A third stage investigated the effect of VKD on an existing groundwater model of the South West Chilterns (Environment Agency, 2000). This stage of the project has been undertaken as part of a wider project entitled 'Enhancements to Modflow' of which the work documented in this report forms the first part.

The enhancements that have been made to MODFLOW have been based on modelling work undertaken at Birmingham University (Rushton & Rathod, 1980, Rushton et al, 1982, Rushton et al, 1989, Rushton & Fawthrop, 1991, and Cross et al, 1995). Many Environment Agency personnel have provided assistance and insight during the various stages of the project, and this is acknowledged.

1.2 Objectives

The objectives of this stage of the project were to take the modified MODFLOW-VKD code produced in Stage II of the project (Environment Agency, 1999) and make the following modifications:

- Allow variation of hydraulic conductivity with depth (VKD) in any model layer (including layers that can become confined).
- Allow variation of specific yield with depth (VSD) in any model layer (including layers that can become confined).
- Make any necessary changes to the auto-conversion routine (which converts normal MODFLOW layers to VKD layers).

In the course of the project some additional code changes were also requested and incorporated into the code. These were:

- Allow a maximum hydraulic conductivity and/or specific yield to be specified for each model cell.
- Make changes to the stream routing package to allow discharges, abstractions or tributary inflows to be specified at any stream node.
- Include an output of model progress to the screen when using the PCG solver package.
- Allow binary output files to be in the same format as those required by Groundwater Vistas (GV – Environmental Simulations Inc, 2001), the Agency's preferred MODFLOW user interface.
- Include an option to allow the input of X- and Y-direction transmissivities or hydraulic conductivities independently (without using the anisotropy ratio method).
- Include the option to allow convergence to be forced if the convergence criteria are met for a specified number of outer iterations (this was not thought to be a particularly useful option, but was included to make the code compatible with models produced by GV).
- Allow a debugging option for the PCG solver so that the evolution of head values at each iteration could be examined – to identify problem areas in models that do not converge.

These changes to the code were then tested to ensure that the code behaved correctly. This testing was to be undertaken both with test models and operational models representing real case studies. Testing the code in the development of operational models was intended to reveal issues that would be encountered in the future, and allow these issues to be addressed.

1.3 Structure of report

The following section provides an overview of the observed behaviour of groundwater in chalk aquifers, and its relationship to varying hydraulic properties with depth. This is followed by a description both of how the modifications that have been made to MODFLOW, and of how these modifications have been tested using various groundwater model simulations. The final section presents the summary, conclusions and recommendations.

2 FLOW PROCESSES IN CHALK AND LIMESTONE AQUIFERS

2.1 Introduction

The nature of chalk and limestone formations, with fluid flow mainly through discrete, solution-enhanced fissures, results in low-storage, highly transmissive aquifers that respond very rapidly to recharge and pumping. The fissures that provide the major resource for these aquifers are more developed in river valleys, where transmissivities and flow rates are higher. These fissures can also provide a good hydraulic connection between the aquifer and surface water, with ephemeral streams and swallow holes a common feature of these catchments. The groundwater flows through fissures which are enhanced by the dissolution of carbonate by recharge (or runoff) waters which are initially undersaturated with regard to calcite. These waters are incident on the water table at the top of the saturated zone, and dissolution and fissure enlargement are therefore concentrated in the zone of fluctuation of the water table (Foster & Milton, 1974; Allen et al, 1997; Price et al, 1993).

Evidence for this variation in properties with depth comes from a number of sources including observation of fissure occurrence and character with depth, analysis of pumping tests, analysis of the seasonality of river flows and analysis of aquifer response to drought and flood episodes.

2.2 Occurrence of fissures

Some of the first work on fissure distribution with depth in the Chalk was undertaken by Thames Water in 1975 (Robinson, 1975). This work describes the evidence for variation of permeability with depth from flow logging, concluding that in unconfined chalk fissures occur mainly from the water table to some critical depth, regardless of geology. The exception was found to be the Chalk Rock which appears to yield water regardless of depth of burial (except in the confined chalk). In confined chalk all major contributing fissures occurred between the base of the well casing and 65 m into the Upper Chalk (displaying a more even distribution of fissures over this thickness than observed in the unconfined chalk). CCTV of several boreholes provided a detailed description of the fissuring.

Figure 2.1 shows the results from analyses of caliper logs from 67 boreholes in the Upper Lee chalk groundwater catchment in Hertfordshire (WS Atkins, 2001). Each metre section of each of the logs was examined to see if there was a discrete increase in the borehole diameter in that interval. Although an increase in calliper log diameter is not in itself proof of the presence of a fissure, the majority are related to fissures and those which are not are unlikely to increase in frequency with depth. Increases of <50 mm were ignored while increases of 50-100 mm, 100-200 mm and >200 mm were given different classifications and entered into a spreadsheet.

A simple plot of the number of fissures versus depth would be biased to shallow depths because shallow depths will be penetrated by both shallow and deep boreholes but greater depths will only be penetrated by deep boreholes. To reduce this bias, the percentage frequency of fissures was calculated for every metre penetrated (and uncased) and a percentage frequency versus depth plot generated based on a 5 m moving average. This analysis reveals a reduction in fissure frequency with depth, which is particularly evident for the larger fissures.

2.3 Pumping tests

One of the easiest ways to illustrate the variation of hydraulic properties with depth is to examine pumping test results from a single borehole, tested at different times of year when the water table is at different elevations. Figure 2.2 shows results from two such tests of a borehole located towards the top of a dry valley in the Berkshire Downs (Rushton & Chan, 1976). The tests were conducted in 1974. The first test was conducted in May, the second in July, with the rest water level 7.5 m lower than in the first, and with a lower pumping rate. Despite the lower pumping rate, the drawdown in the second test became excessive after 6 days and the pump was switched off.

In itself, the fact that the second test resulted in excessive drawdown at a lower pumping rate suggests that the upper part of the aquifer supplies a significant proportion of the water. Using traditional pumping test analysis of levels in an observation borehole, two different values of transmissivity of 400 and 190 m^2/d were obtained for the first and second tests respectively. In addition, the steepening of the drawdown curve for the first test suggests that the transmissivity reduces significantly with depth.

If the results of several pumping tests are analysed to give a value of transmissivity and storage for different rest water levels, a profile of the variation of aquifer properties with depth can be plotted. Figure 2.3 shows the results of a series of pumping tests, analysed using conventional methods, for the Hampshire Chalk (Headworth et al 1982) and the London Basin Chalk (Owen, 1981). The plots clearly show a non-linear relationship between transmissivity and rest water level, with transmissivities reducing dramatically below the normal 'zone of fluctuation' of groundwater heads. The plots show that the storage coefficient also changes with the rest water level.

2.4 River flows

The large increases in transmissivity associated with high groundwater levels mean that groundwater can move through the aquifer at much greater rates in winter and spring when the water table is high, than during the summer when levels are low. Combined with good hydraulic connection to surface water, this leads to large seasonal variations in the flow in groundwater-fed rivers, as can be seen in the River Bourne in Figure 2.4 (Environment Agency, 2001). Often, many streams and smaller rivers will dry up completely during the summer months. Accurate simulation of river flows is an important requirement for regional groundwater models, and it was the difficulties encountered with this aspect of modelling that has led to the development of modelling codes that allow hydraulic conductivity to vary with depth.

2.5 Responses to drought and flooding

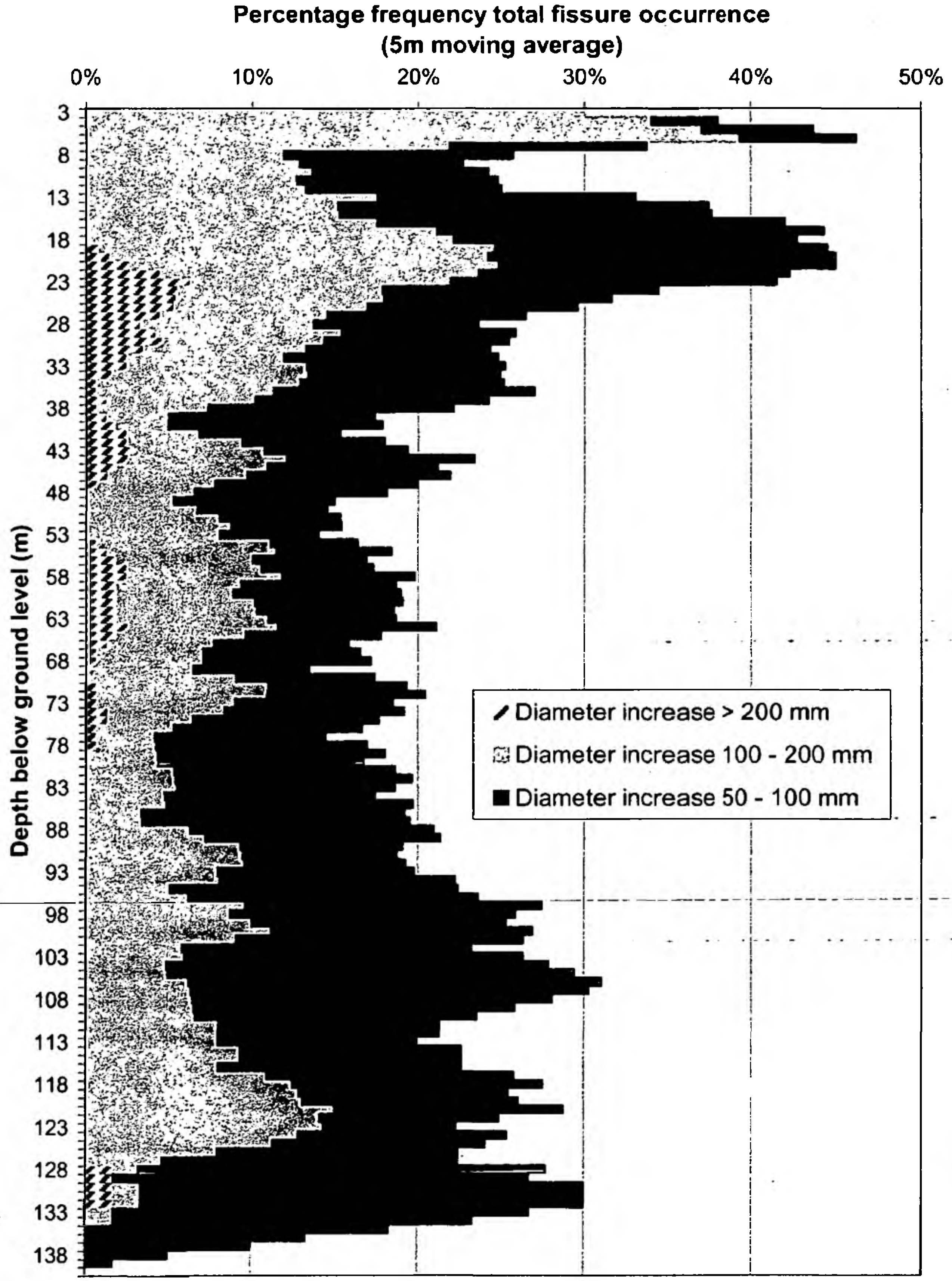
Another effect of the large variations in hydraulic properties with depth is that once the water table falls below the normal zone of fluctuation, levels can drop dramatically. This effect can be seen in years 1989 and 1990 in Figure 2.5, which shows a groundwater hydrograph from the Southwest Chilterns (Environment Agency, 2000). Equally, when the system is subsequently recharged, levels can rise very sharply (1992 in Figure 2.5).

The recent floods in Southern Region have revealed some interesting properties of the chalk when groundwater levels are high. Groundwater hydrographs in the South Downs and around the Isle of Wight have shown a sudden increase in groundwater heads once they had risen above the normal maximum. This suggests that specific yield and/or hydraulic conductivity may reduce again above the normal 'zone of fluctuation' of groundwater heads.

This configuration could be incorporated into the VKD code, but the present coding, involving gradient factors and the auto-conversion option, could prove to be difficult to use. A reduction in specific yield/hydraulic conductivity at higher elevations was considered to be too complicated to be included in the code at this stage.

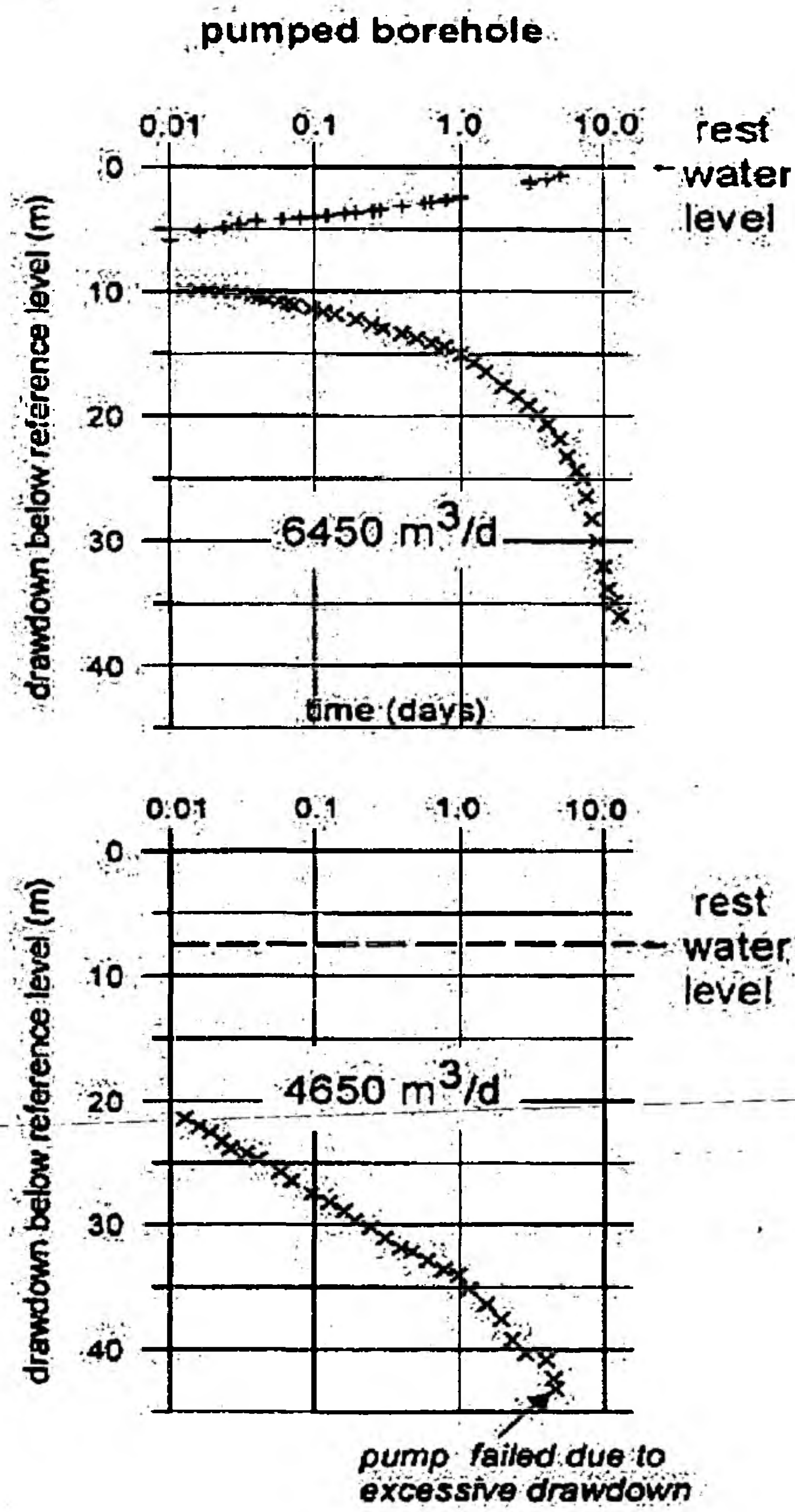
WATER MANAGEMENT CONSULTANTS

Figure 2.1 Observed variation of fissure frequency with depth from caliper logging in the Upper Lee catchment



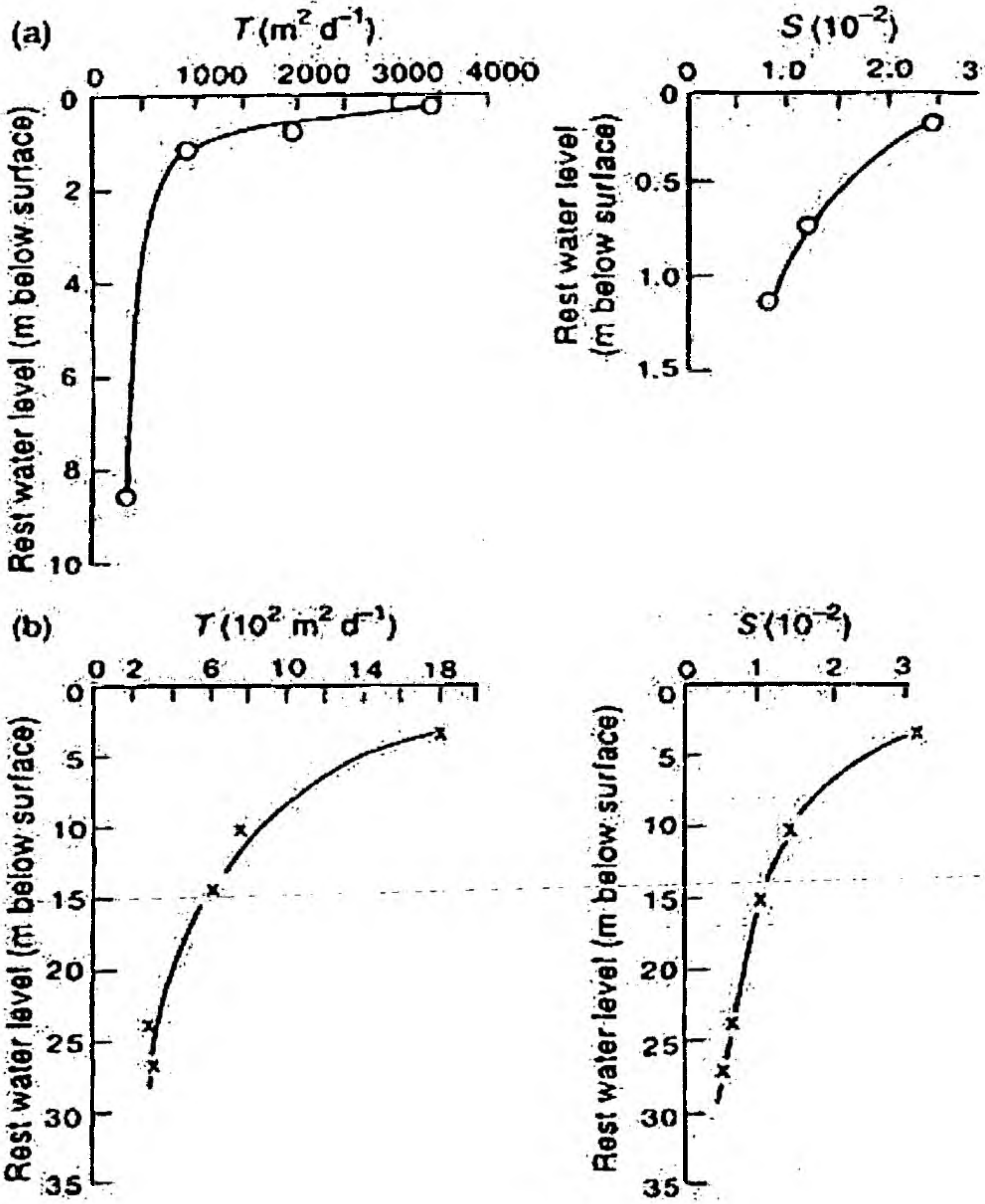
WATER
MANAGEMENT
CONSULTANTS

Figure 2.2 **Pumping test results from a single borehole, tested at different times of year (Rushton and Chan, 1976)**



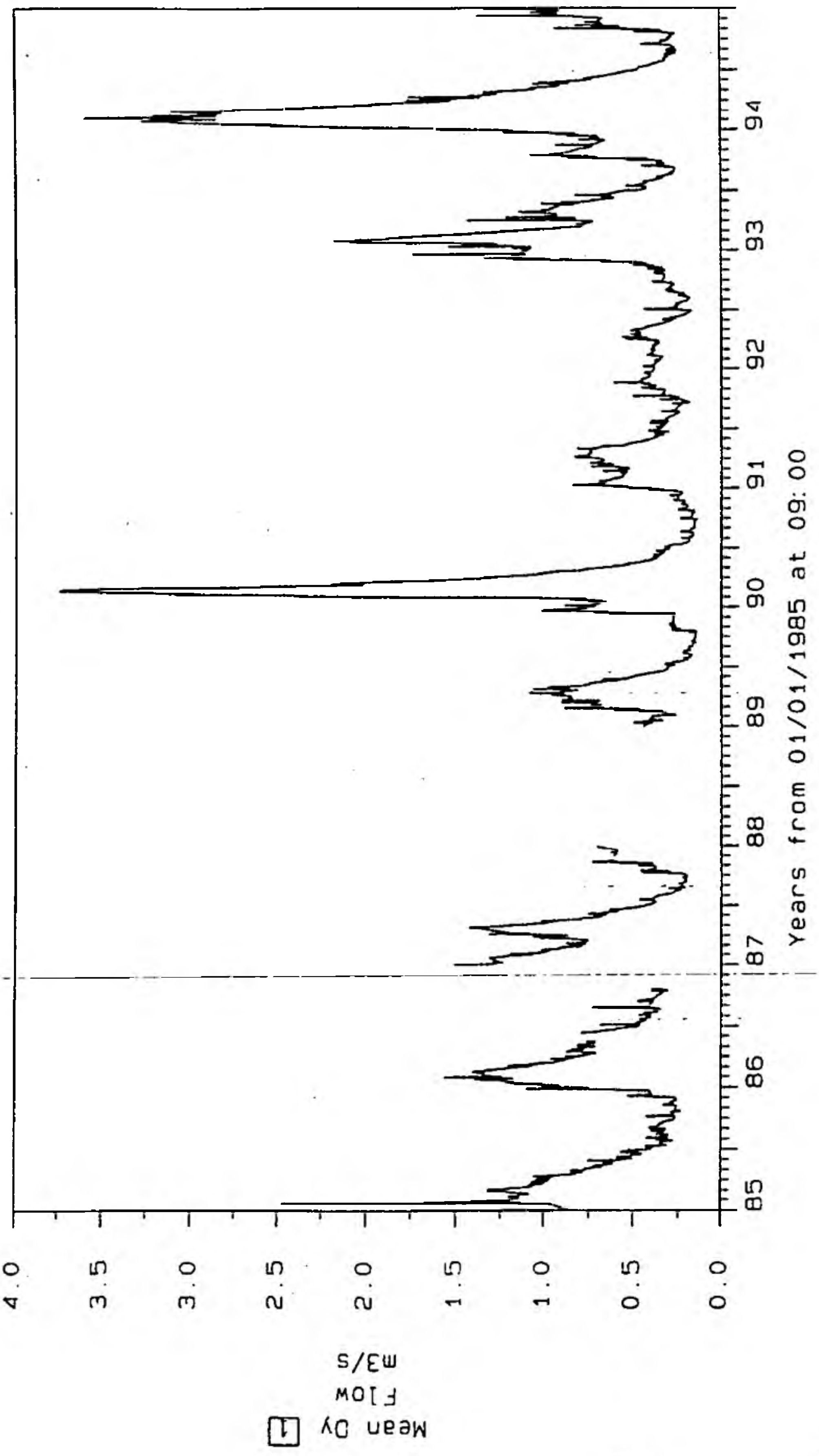
WATER MANAGEMENT CONSULTANTS

Figure 2.3 **Observed changes in transmissivity and storage with depth (Headworth et al. 1982 & Owen 1981)**



WATER MANAGEMENT CONSULTANTS

Figure 2.4 Hydrograph for the River Bourne showing large variations in flow (Environment Agency, 2001)



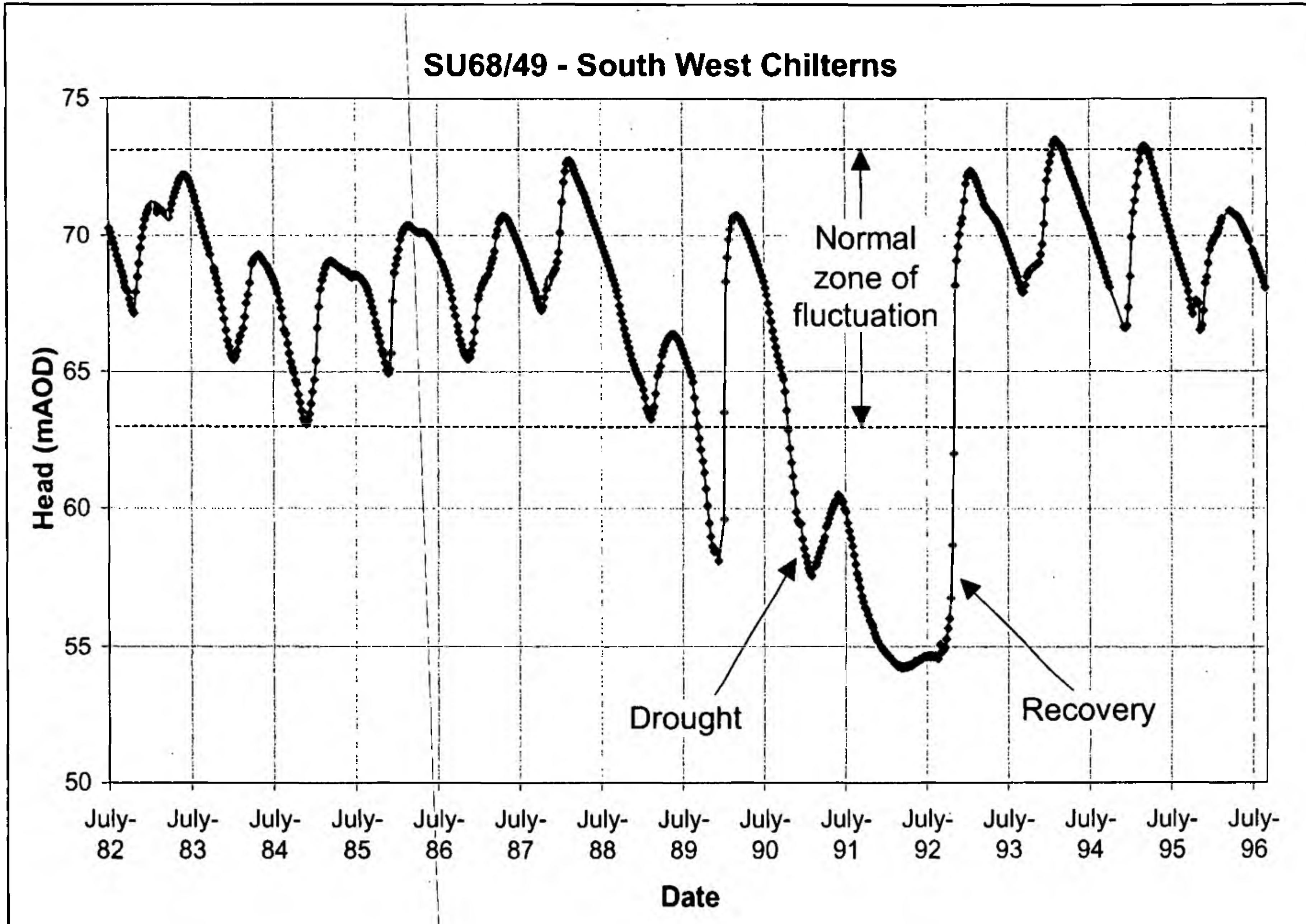


Figure 2.5 Groundwater hydrograph showing abrupt changes in groundwater level during droughts

3 MODIFICATIONS TO THE MODFLOW CODE

3.1 Introduction

Traditionally, chalk and limestone aquifers have been represented in groundwater models as a thin layer representing only the 'active flow zone', which is usually assumed to be between 30 and 60 m thick, with no variation of hydraulic conductivity with depth. These constant hydraulic conductivity models give rise to a linear variation of transmissivity with depth, which is a poor approximation to observed behaviour (Section 2). The limited representation of the conditions in the aquifer means that, in order to represent observed behaviour, the modeller may need to employ unrealistic or contrived values for other model parameters such as storage, river conductance, or temporal distribution of recharge.

An additional problem with these types of MODFLOW models is that if a severe drought is being simulated, groundwater heads can fall below the normal active flow zone, resulting in cells becoming 'dry', and distorting the pattern of flow. If a low hydraulic conductivity layer is added below the active flow zone to enable 'wetting' of the layer above, the contrast in hydraulic conductivity between the two layers often results in numerical oscillations as cells change between wet and dry, reducing the likelihood that the model will converge.

3.2 Previous work

In order to simulate more accurately the flow processes observed in the Chalk, the MODFLOW code was modified such that hydraulic conductivity could vary with depth (Figure 3.1, Environment Agency, 1999 & 2000). The resulting simulated non-linear relationship between transmissivity and groundwater level approximates that of the observed relationship shown in Figure 2.3.

This kind of relationship was first included in groundwater models of the chalk constructed at the University of Birmingham, including models of East Kent (Cross et al, 1995), the Berkshire Downs (Rushton et al, 1989), Candover (Rushton & Rathod, 1980), and Lincolnshire (Rushton et al, 1982). The modified MODFLOW code was tested against the Birmingham code using a number of purpose-built test models. Additional investigations have been undertaken to assess the effect of inclusion of variable hydraulic conductivity with depth in an existing model of the Southwest Chilterns (Environment Agency, 1999 & 2000).

3.2.1 Effect of VKD on simulation results

Figure 3.2 shows a comparison of the modelled base flows in the River Wye, from the Chilterns model. The dashed line shows the response of the original model, which uses a constant hydraulic conductivity with depth. The solid line shows the response from a version of the same model, which allows variation in hydraulic conductivity with depth (VKD). This figure shows that, although the two models have the same sequences of recharge and the same storage coefficients, the baseflow in the river is more variable in the VKD model than it is in the constant hydraulic conductivity with depth model.

Figure 3.3 shows an observed groundwater hydrograph compared with outputs from the models described above. In this case it can be seen that the VKD model produces less variation in the groundwater heads, giving a better match with the observed response.

Although the variation in heads is reduced, the variation in transmissivity is increased due to the shape of the hydraulic conductivity profile. It is this profile that enables the VKD model to reproduce large variations in flow, whilst reducing the variation in groundwater heads.

3.2.2 Additional modifications to the MODFLOW code

The non-linear relationship between transmissivity and groundwater level (Figure 3.1) can result in numerical instabilities and non-convergence in some simulations. This is especially true for steady state simulations, if the initial heads are very different from the eventual solution. For this reason, a methodology was developed to significantly reduce the likelihood of instabilities (This method is not always necessary – see Section 4.3.4 on the Upper Lee groundwater modelling project). This methodology consists of three steps:

Step 1. Construct a simplified steady-state model. This model does not include variations in hydraulic conductivity with depth, but instead uses specified transmissivity values (or constant k with depth parameters) to characterise the aquifer. All the other features of the model, such as boundary conditions, are also included in this model. This simplified model can be refined to obtain an adequate agreement between modelled and observed heads and flows.

Step 2. Once the simplified model has reproduced the observed heads and flows to an acceptable degree, VKD parameters are calculated that give the same transmissivity values used in Step 1, when the groundwater heads are at the levels calculated by the simplified model. These parameters describe the variation of hydraulic conductivity with depth (Figure 3.1), and many different combinations of parameters can give the same transmissivity value for a given groundwater head. Although the choice of VKD parameters will not affect the steady state solution, they will affect subsequent time-variant simulations. The choice of VKD parameters should be based on the hydrogeological understanding of the area.

Step 3. The steady-state model is then re-simulated using the VKD parameters calculated in Step 2, and using the heads calculated in Step 1 as the initial conditions. The results of this simulation should be identical to those from Step 1.

Once these three steps have been successfully completed, time-variant simulations can be undertaken, using the heads from the steady-state model as initial conditions. The VKD parameters chosen in Step 2 will have an effect on the results of the time-variant simulation.

The procedure described above was included in the modified MODFLOW code to enable efficient calculation of VKD parameters and to produce data files which can be used as a basis for creating input files for time-variant simulations.

In addition to the features described above, the code was also modified to include the following features:

- Spatially variable anisotropy (Kladias & Ruskauff, 1996).
- Inter-nodal transmissivity option.
- Option to allow input of X- and Y-direction transmissivities independently.
- Explicit transmissivity calculation option.
- Output of calculated transmissivity values to the output file.

The modified MODFLOW code is completely backward compatible with MODFLOW-96.

3.3 New modifications

3.3.1 Introduction

The modifications reported here were made to make the code more versatile. Principal among these modifications were those to allow variation of hydraulic conductivity with depth in any model layer (previously only the upper layer could have VKD) and those to allow variation of specific yield with depth. Additional modifications were also made to the stream routing package, the PCG solver and the utilities package. A full description of the changes made to the code is included in Appendix A. The code with all the changes highlighted can be found in the appendix to the User Guide (Environment Agency, 2002).

3.3.2 Modifications to the Block Centred Flow (BCF) Module

The Block-Centred Flow (BCF) package (Harbaugh & McDonald, 1996) computes the conductance components of the finite-difference equation, which determines the flow between adjacent cells. It also computes the terms that determine the rate of movement of water to and from storage. To make the required calculations, it is assumed that the node is located at the centre of each model cell.

Modifications were made to this package to extend the VKD capabilities to any model layer, and also to allow variations in storage with depth in any layer. This included making changes to the auto-conversion routine for converting standard MODFLOW layers to VKD layers. In addition, some other minor changes were made to the available inputs and outputs.

Multiple layers with variation in hydraulic conductivity with depth

This capability was achieved by including an additional Layer-type (LAYCON) value. Layer-type 4 continues to be used to specify an unconfined VKD layer in the uppermost layer. The new Layer-type, 5, is used to specify a VKD layer with a top that can be confined or unconfined, depending on the groundwater head. This Layer-type can be specified for any layer in the model.

A maximum value for the hydraulic conductivity can now be specified for the upper part of the hydraulic conductivity profile (VKMAX array). The maximum hydraulic conductivity is specified as a multiple of the base hydraulic conductivity. This means that any anisotropy specified for the base hydraulic conductivity is also reflected in the maximum hydraulic conductivity. Specifying the maximum hydraulic conductivity as a multiple of the base hydraulic conductivity (rather than as an independent value) also makes the maths involved in the auto-conversion calculations simpler.

The transmissivity for each cell is calculated during each iteration from the following properties (see Figure 3.4):

Base hydraulic conductivity, k_{base} [LT^{-1}]
Bottom elevation, e_{bot} [L]
Elevation of point of inflection, e_{mid} [L]
Hydraulic conductivity gradient factor, f [L^{-1}]
Maximum hydraulic conductivity factor, k_{max} [-]
Top elevation, e_{top} [L]
Groundwater head, h [L]

The elevation (e_{kmax}) where the hydraulic conductivity reaches its maximum value is given by:

$$e_{kmax} = e_{mid} + \frac{k_{max} - 1}{f}$$

Equation 3.1

The transmissivity is calculated in different ways depending on the elevation of the groundwater head within the hydraulic conductivity profile. If the head is below the point of inflection then the transmissivity, T, [L^2T^{-1}] is simply:

$$T = k_{base}\left(h - e_{bot}\right)$$

Equation 3.2

If the head is above the point of inflection but below the elevation where the hydraulic conductivity reaches its maximum, then the following relationship is used:

$$T = k_{base}\left(h - e_{bot}\right) + \frac{k_{base} f \left(h - e_{mid}\right)^2}{2}$$

Equation 3.3

If the head is above the elevation where the hydraulic conductivity reaches its maximum, the transmissivity is given by:

$$T = k_{base}\left(h - e_{bot}\right) + \frac{k_{base} f \left(e_{kmax} - e_{mid}\right)^2}{2} + k_{base}\left(k_{max} - 1\right)\left(h - e_{kmax}\right)$$

Equation 3.4

If the groundwater head is above the top of the layer (for Layer-type 5 only) then Equation 3.4 is used with the groundwater head, h, replaced by the top elevation, e_{top}.

If the groundwater head is below the bottom elevation, then the cell becomes inactive (dry) in the same way as for Layer-types 1 and 3.

The code checks the hydraulic conductivity gradient factor array for zeros (conceptually this would mean no variation of hydraulic conductivity with depth for the cell concerned, but it results in a divide by zero error in the transmissivity calculations). Any zero or negative values are replaced by an arbitrary number (one), and the maximum hydraulic conductivity factor for that cell is set to one. This also produces no variation of hydraulic conductivity with depth. These cells are reported to the output file.

Variation of storage with depth (VSD)

The code was updated to include variation of specific yield with depth (VSD). The shape of the storage profile is controlled in a similar way to that of VKD, using a gradient factor and a maximum factor (see Figure 3.5).

Problems have been encountered with convergence in simulations using VSD. These are thought to be due to a necessary approximation in the code, which assumes small changes in groundwater heads between iterations. For this reason it is suggested that this capability should be made inactive (by setting the gradient factor to zero or the maximum factor to one) unless the field evidence indicates that it is an important feature of the catchment. If this is the case, problems with convergence may be reduced by applying one (or more) of the following suggestions:

- Using a low value for the storage gradient factor so that there are only small changes in storage with depth.
- Using a high value for the storage gradient factor and set the maximum storage factor at a value such that the interval over which storage changes is small.
- Decreasing the size of the time steps used in the simulation.
- Finding optimum solver parameters to solve the problem (eg set the maximum inner iterations for the PCG2 solver to 1 or 2 and try both the preconditioning methods).

Modifications to the auto-conversion routine

A number of changes were made to the auto-conversion routine. These included:

- An additional option to allow conversion of constant hydraulic conductivity layers to VKD layers. This is achieved by setting the steady state flag (ISS) to 3 and entering vertically averaged horizontal hydraulic conductivities instead of transmissivities. The original option to specify transmissivities is still activated by setting the steady state flag to 2.
- Changes to the inputs required for the auto-conversion option. It was agreed that bottom elevations for the layer would be used rather than a thickness for the lower part of the layer. This allows the elevations of divisions between layers to be input directly and avoids the likelihood of producing overlapping layers. The calculated thicknesses of the lower zone (constant hydraulic conductivity) are printed to the output file.

- Specification of the thickness of the varying hydraulic conductivity zone rather than the elevation of the base of this zone. It was thought that the user would have a better idea of the thickness of this zone rather than the elevation of its base.

- If the head calculated in the first simulation is less than the specified upper thickness above the base of the layer, the upper thickness is automatically adjusted to be equal to the difference between the head and the bottom elevation. The lower thickness is then set to zero. A message is printed to the output file for each cell where the upper thickness has been adjusted (and where the lower thickness is zero), and the array of upper thicknesses is also printed.

It should be noted that for the automatic-conversion process the user now specifies 1) transmissivity, 2) upper thickness, 3) bottom elevation, 4) hydraulic conductivity gradient factor (F), 5) top elevation if the layer is confined, & 6) the maximum hydraulic conductivity factor. The code calculates 1) groundwater heads, 2) elevation of point of inflexion (head – upper thickness), 3) bottom thickness (point of inflexion – bottom elevation) & 4) Kbase (Figure 3.6).

In relation to the automatic calculation of VKD parameters, it is emphasised that the values of Kbase calculated by the code (written to the second BCF file) should be checked by the user to make sure they are realistic. These values could then be adjusted by the user and sorted into zones (rather than having a different value of Kbase for every cell).

Handling of dry cells

The way the auto-conversion routine handles dry cells has also been revised. Originally the code performed the first simulation by changing the layer type from VKD (LAYCON = 4 or 5) to confined (LAYCON = 0), using the values of transmissivity specified by the user. The problem with this approach is that when LAYCON is zero, the code does not check the calculated heads against the bottom elevation, and all the cells remain active regardless of whether heads are above or below the bottom of the layer. This meant that when the second simulation started, cells in which heads were below the bottom elevation became inactive, and the flow field changed.

To remedy the above, the code was changed so that the layer type remained the same (LAYCON = 4 or 5), but that the transmissivity calculation was changed if the automatic conversion option was specified (ISS = 2 or 3). This allows the code to check the heads against the bottom elevation, and so make the cell dry if the head falls below the bottom of the layer. In this way, if the steady state flag is set to 2, the transmissivity of each cell is set to a constant value, unless the head falls below the bottom in which case it is set to zero. (It should be noted that if a confined layer type is specified by the user (LAYCON = 0), the code behaves in the same way as the standard MODFLOW96 code.)

A number of additional issues have been raised in relation to the problem of dry cells:

- In order to avoid unrealistic initial heads for the second simulation, the dry cell value (HDRY) should be set to an elevation below the bottom of the lowest cell in the model (recommend using HDRY = -888). This ensures that this cell will remain inactive in the second simulation.
- If rewetting is active, the dry cell value should be set to a different value than the no-flow cell value (recommend -999).
- As the automatic calculation of VKD parameters does not work for cells that have become inactive, the following changes were made:
- All property values at no-flow and dry cells are set to zero in the second simulation. This means that if, in a subsequent simulation, the rewetting option is activated, and inactive cells are allowed to become active again, the zero properties will mean that the cell becomes immediately inactive again (MODFLOW automatically makes a cell inactive (head = 888.88) if it has zero conductances to all its surrounding cells). If a cell is required to rewet in a simulation (assuming heads will rise and rewet the cell) alternative VKD properties should be specified manually for that cell by the user.
- To avoid the problem of rewetting inactive cells, it is suggested that the initial heads for time variant simulations should be obtained for an instant in time when groundwater heads are at their maximum (using the time-instant approach – see Section 4.2.1).

Formats of arrays

The code was changed so that the user does not have to specify a high degree of precision in transmissivity and upper thickness values in order to produce good agreement between the first and second simulations. The format codes used for writing the base hydraulic conductivities and elevations of the points of inflection to the second BCF file (which have a large influence on the transmissivity calculations) are automatically set to a high degree of precision (rather than being the same as the input formats for transmissivity and upper thickness, as was previously the case).

The code that writes the new BCF and BAS packages was also changed to check if all (active) values in an array are equal, and if so, a constant array record is written, rather than writing values for all cells, thus saving disk space.

Filenames

The auto-conversion routine produces additional MODFLOW input files for the basic (BAS) and block-centred flow (BCF) packages, which are used as part of the input for the second simulation. Previously the filenames for these files were based on the original filenames with the last character changed to a '2' (eg 'Run1.bcf' becomes 'Run1.bc2' in the second simulation). The same was true for the output files from the second simulation (eg 'Run1.lst' and 'Run1.hds' are changed to 'Run1.ls2' and 'Run1.hd2') This has now been changed so that the user can specify their own filenames for these files in the 'name file'. For each relevant file, the filename for the second simulation is entered on the same line as that for the first, separated by any number of spaces and a '>' character. For example, the line in the name file which specifies the name of the BCF file can now be written as follows:

BCF 11 Run1a.bcf > Run1b.bcf

where 'BCF' defines the file type, '11' is the unit number that the file will be opened under, the first filename is the name of the input file created by the user, and the second filename is given to the BCF file created at the end of the first simulation.

Additional modifications

X- and Y-direction transmissivities/hydraulic conductivities

A minor modification was made so that if X- and Y-direction transmissivities or hydraulic conductivities are input independently (ITRPY=2), the actual values are stored in the arrays rather than the anisotropy ratios being calculated internally. The main difference this makes is that zero values can be entered for X- direction properties without producing a 'divide by zero' error.

Output of leakance values to the listing file

The option that was added to allow an output of inter-nodal transmissivity values to the listing file has been modified so that, if the option is chosen, vertical leakance values between layers are also printed.

3.3.3 Modifications to the Stream Routing module

The Streamflow-Routing (STR) package (Prudic, 1989) is a modification of the River Package (McDonald & Harbaugh, 1988 and Harbaugh & McDonald, 1996) designed to route flow through one or more rivers, streams, canals or ditches (hereafter referred to as streams) in addition to computing the leakage between the streams and the aquifer system.

Modifications were made to this package to allow surface water discharges or abstractions to be specified at any stream cell and to allow tributary inflows to be allowed at any reach in a stream segment. In addition, a small correction was made to the cell-by-cell stream flow output.

Specified discharges or abstractions at any stream cell

The original version of the stream package allows an inflow to be specified only for the first reach (ie first cell) of a segment. This inflow can either be the calculated stream flow from one or more upstream segments or it can be a specified flow rate. The input format includes a column for this flow rate for all stream reaches, but the value was ignored in all but the first reach in each segment. It appears that the original version of the package was intended to allow inflows at any cell but that this was later changed.

The revised version of the stream package allows the user to specify additional discharges or abstractions at any reach of any stream segment. This means that contributions to surface water flow from discharges or runoff can be specified at any stream cell. The use of the –1 flag to denote tributary inflows is no longer used, allowing negative flows (abstractions) to be specified (connections to tributaries are now handled entirely by input block 5 – see the User Guide). If the specified abstraction rate is greater than the flow in the stream, then the abstraction is set equal to the inflow to that reach (drying the reach) and a message giving the reduced abstraction rate is written to the output file. To determine whether this option is used, a new flag (ISWABS) is read from the first line of the input file. This flag should be set to a non-zero value to activate the option.

Tributary inflows at any stream cell

The second modification allows tributary inflows to be specified for any reach in a segment (previously tributary inflows were only allowed in the first reach of a segment). This modification allows a major river to be specified with a single segment number, with tributary inflows from smaller streams at various points along its length. This change has been made to make pre- and post-processing easier. Setting the new flag (ISWABS) to a positive value activates the option.

Correction to the cell-by-cell stream flow output

The final modification was made to the routine that writes the streamflows to the binary cell-by-cell output file. This change only affects simulations where more than one stream reach is defined in a single model cell. This would not normally be done, except perhaps at a confluence. The original version of the stream package summed the total streamflow in all the reaches in the cell and wrote this summed value to the output file, giving an erroneous value for the accreted streamflow at that point. A correction was made to the code so that only the stream flow from the furthest downstream reach was recorded in the binary output file.

3.3.4 Modifications to the PCG2 Solver Package

The Preconditioned Conjugate-Gradient (PCG) Solver Package (Hill, 1990) is one of the more powerful solvers available for MODFLOW. The solver allows a solution to be found that satisfies criteria of both minimum head change and flow residual.

The solver converges on a solution through a series of inner and outer iterations. The coefficients of the finite difference equations (some of which are head-dependent) are recalculated at the start of each outer iteration, based on the current estimate of the head distribution. Within each outer iteration a number of inner iterations are carried out during which the coefficients remain unchanged.

The changes that have been made to this version of the solver package do not affect the way that the finite difference equations are solved.

Progress monitor

The first modification prints convergence information to the screen whilst the model is running so that the progress of the simulation can be monitored. There is no option to disable the progress monitor. The information written to the screen includes the stress period, the time step, the iteration and the current degree of convergence in terms of the head difference and the flow residual.

Forced convergence facility

The original version of the package only reaches convergence if the criteria are met during the first inner iteration of an outer iteration. This means that the convergence criteria can be met at the end of an outer iteration but if the criteria are not met immediately once the coefficients are updated, the iterations continue. The new option allows the user to specify the maximum number of consecutive outer iterations (NOUTC) during which the criteria are met before convergence is 'forced'. This can sometimes lead to large water balance errors.

This modification has been made to make this version of the code compatible with the Windows version of MODFLOW supplied with Groundwater Vistas (the Agency's preferred MODFLOW user interface (Environmental Simulations Inc, 2001)). ***It should be stressed that the use of this option can adversely affect the accuracy of the solutions obtained and it is not recommended that the option be used without great caution and independent checks of the water balance.***

Debugging option

The final modification can be used to identify problem areas in a simulation that fails to converge. To activate the option a unit number is entered at the top of the input file (IPCGDEBUG) and file name specified in the NAME file as DATA(BINARY). The simulation will then produce a heads-type binary output file containing the heads calculated in each iteration. This file is created for every time step of the simulation, and is cleared each time the convergence criteria are met, so only the heads from the unconverged time step remain in the file. It should be noted that this option will slow simulations down and large files can be created. The contents of the file produced are described in the User Guide.

3.3.5 Modifications to the utilities package

The utilities package (Harbaugh & McDonald, 1996) contains routines to read data from, and write data to, data files. Its main functions include reading one- and two-dimensional real and integer arrays, and writing arrays to the output file or to binary files.

Allow use of direct access binary files

The routine in the basic package that opens all the files in the NAME file (SBAS5O) allows the user to specify a binary file as a direct access file by entering the word 'DIRECT' after the filename. A number specifying the record length of the direct access file (in bytes) should follow this keyword (a value of 1 will ensure that the file opens without an error).

This modification to the utilities package allows the head, drawdown and cell-by-cell flow files to be written in direct access format. This is the same format as the files created by the Windows version of MODFLOW (MFWin32) supplied with Groundwater Vistas (Environmental Simulations Inc, 2001) and enables output from the modified MODFLOW code to be processed by Groundwater Vistas. The record length of the file is calculated from the model dimensions when the first record is written, any previous contents of the file are cleared and the file is re-opened with the correct record length. Subsequent records are then added to the file as specified in the Output Control file.

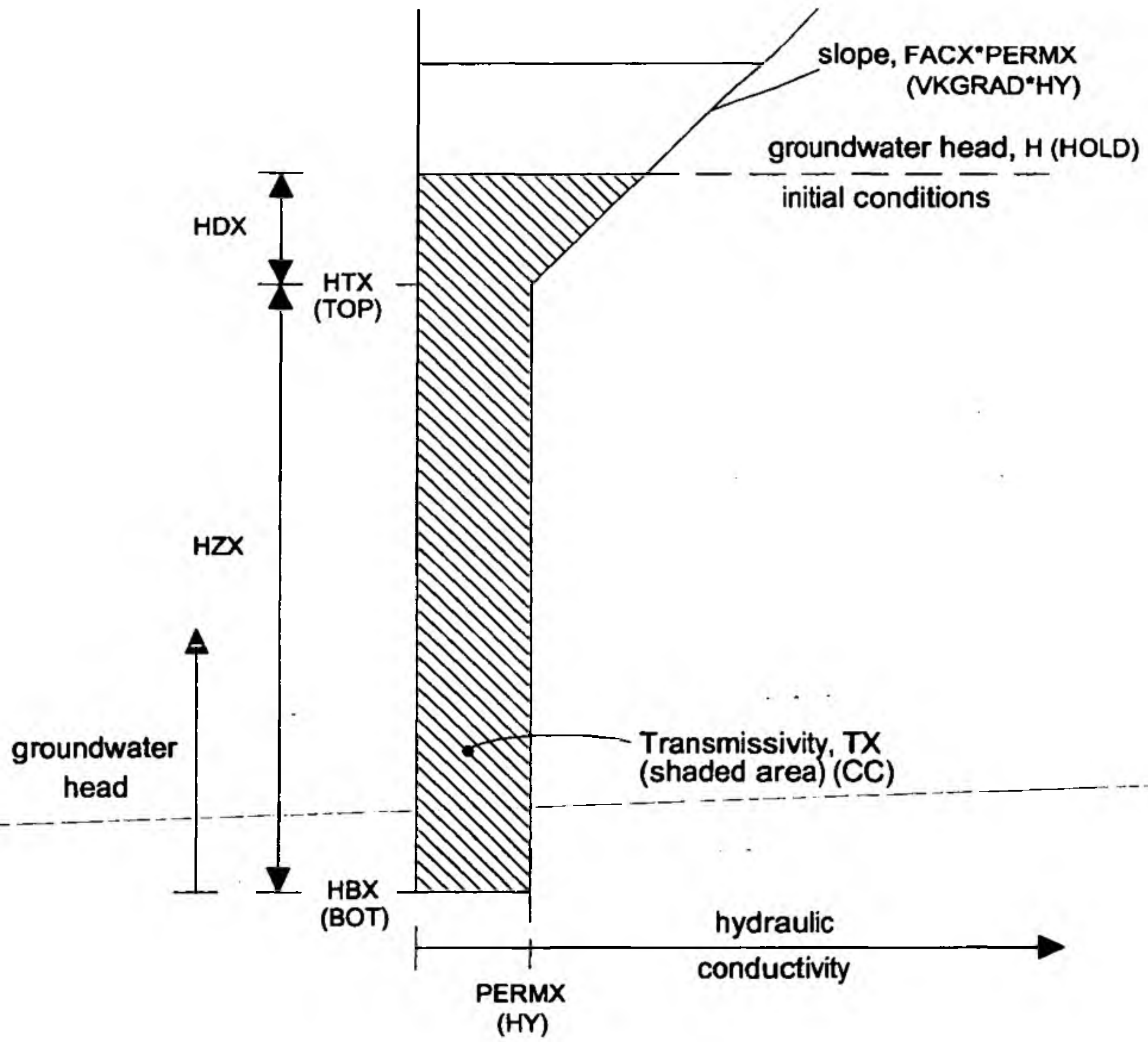
3.3.6 Modifications to the main program

The changes to the main program (MF-VKD1.for) mainly consist of changes to those parts of the code that "call" the subroutines of the modified packages (BCF, Stream and PCG). Other changes that have been made include:

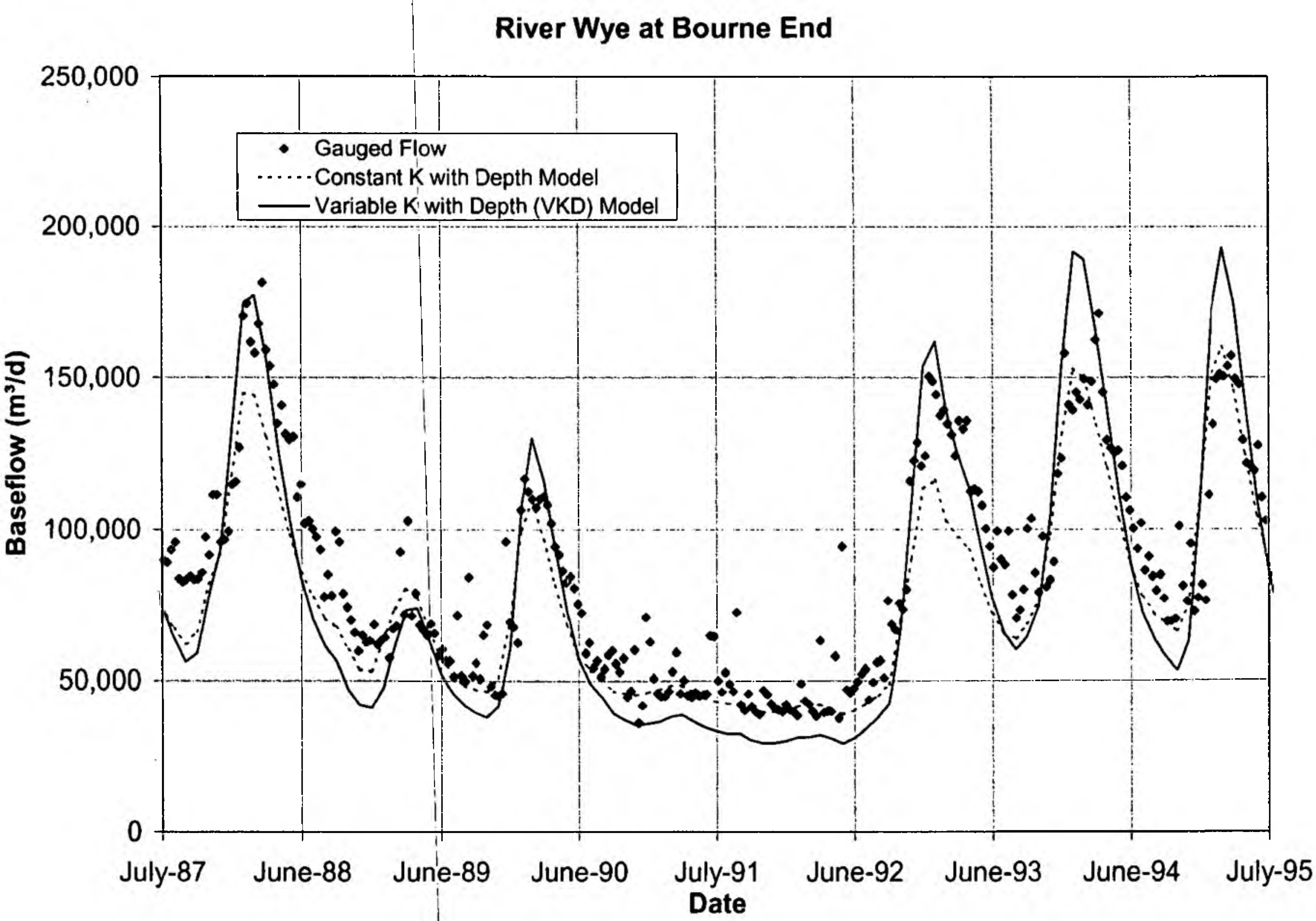
- Increasing the size of the X array from 1,500,000 to 10,000,000. This change increases the total memory requirements of a simulation that uses the entire X array to 38 megabytes. However, use of dynamic storage on many operating systems means that this total is rarely needed.
- Allowing the progress monitor to be printed to the screen when using the PCG solver (see Section 3.3.4).
- Allowing the code to loop back and run a second simulation when using the auto-conversion option (see Section 3.3.2).
- Allowing the output of calculated transmissivity values to the listing file (see Section 3.3.2).

WATER MANAGEMENT CONSULTANTS

Figure 3.1 Numerical simulation of variable hydraulic conductivity with depth

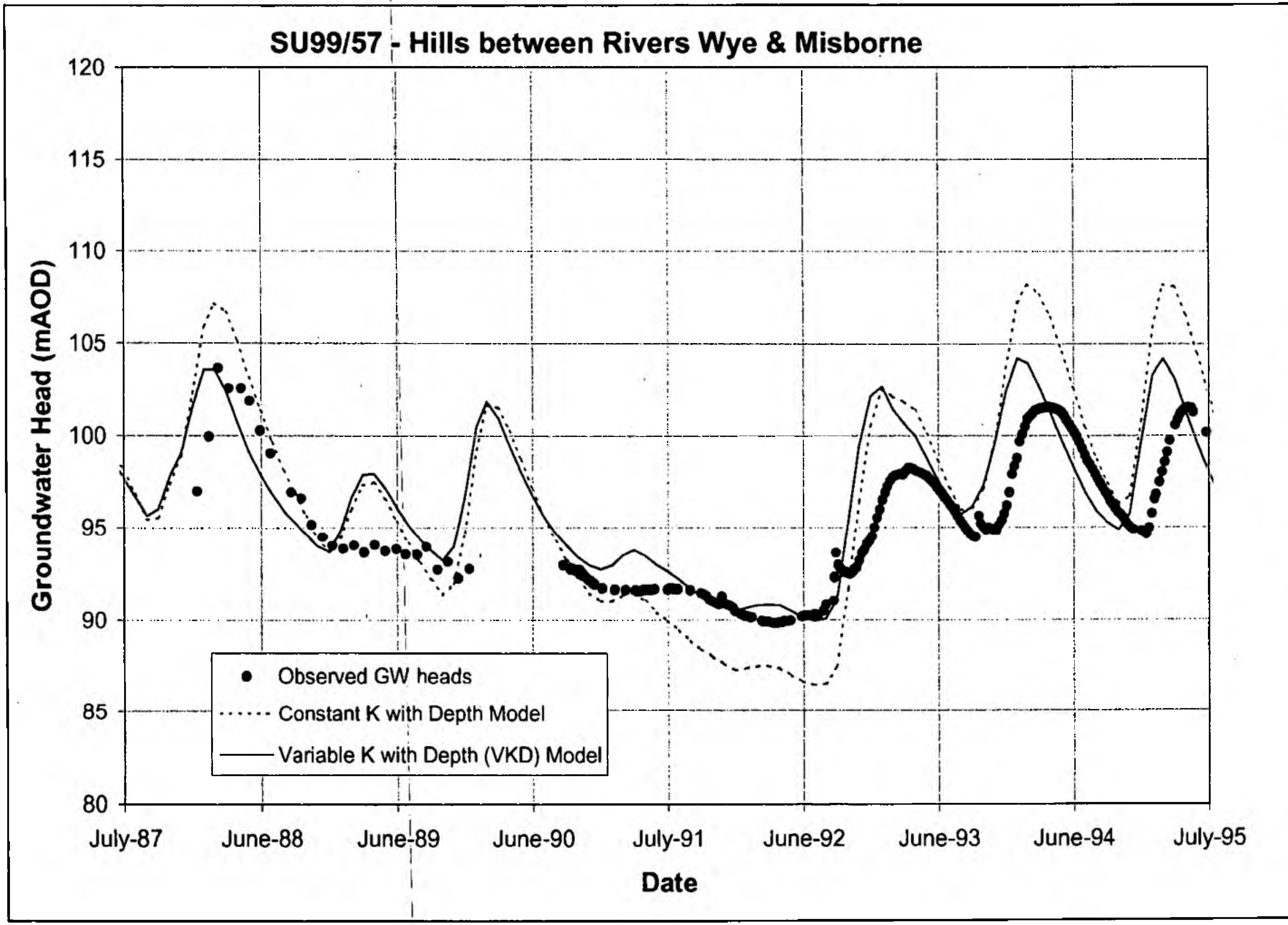


BHM variable name
(MODFLOW variable name)



WATER MANAGEMENT CONSULTANTS

Figure 3.2 Simulated base flows in the Southwest Chilterns groundwater model, with and without VKD



WATER MANAGEMENT CONSULTANTS

Figure 3.3 Simulated groundwater heads in the Southwest Chilterns model, with and without VKD.

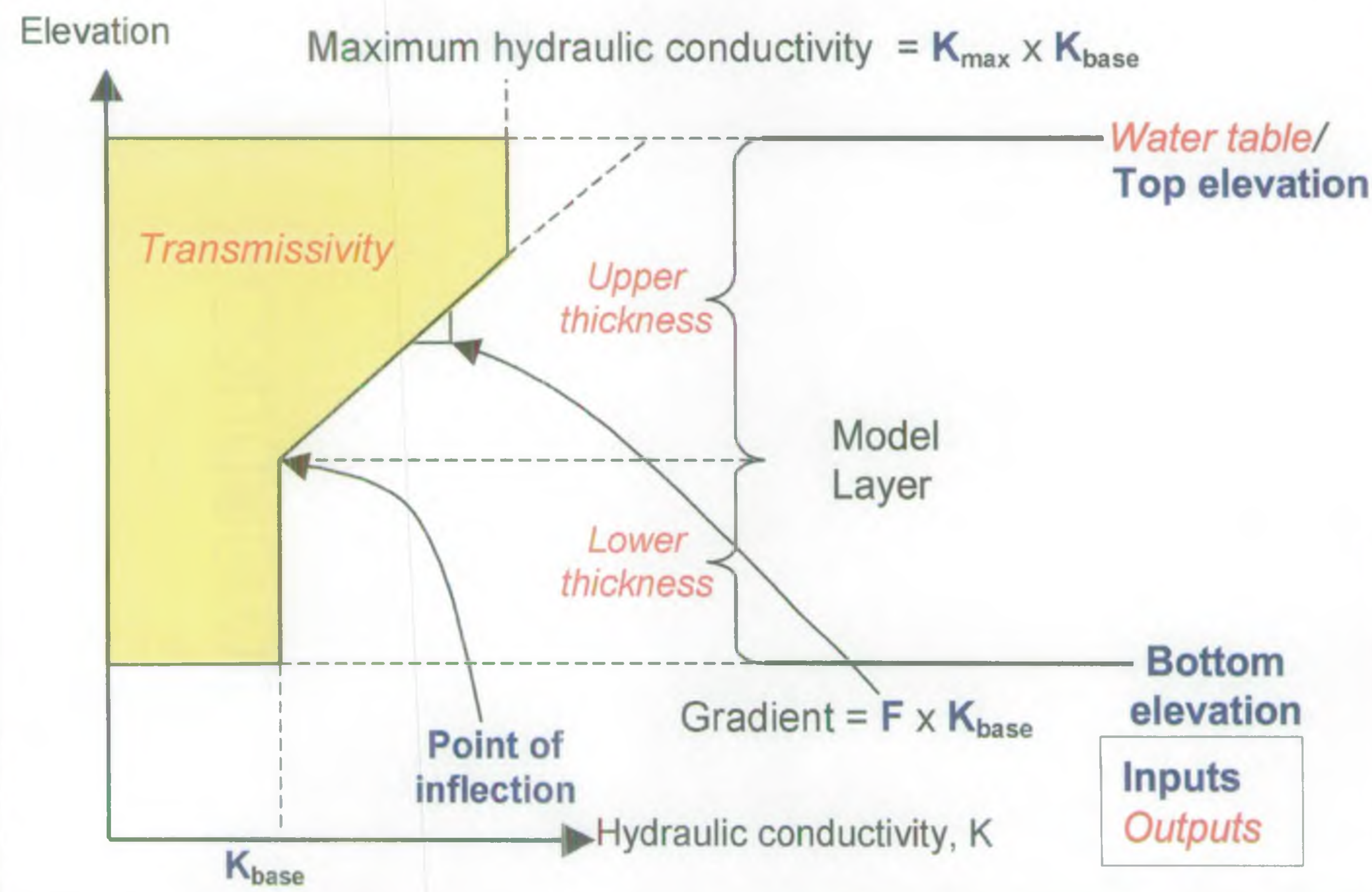
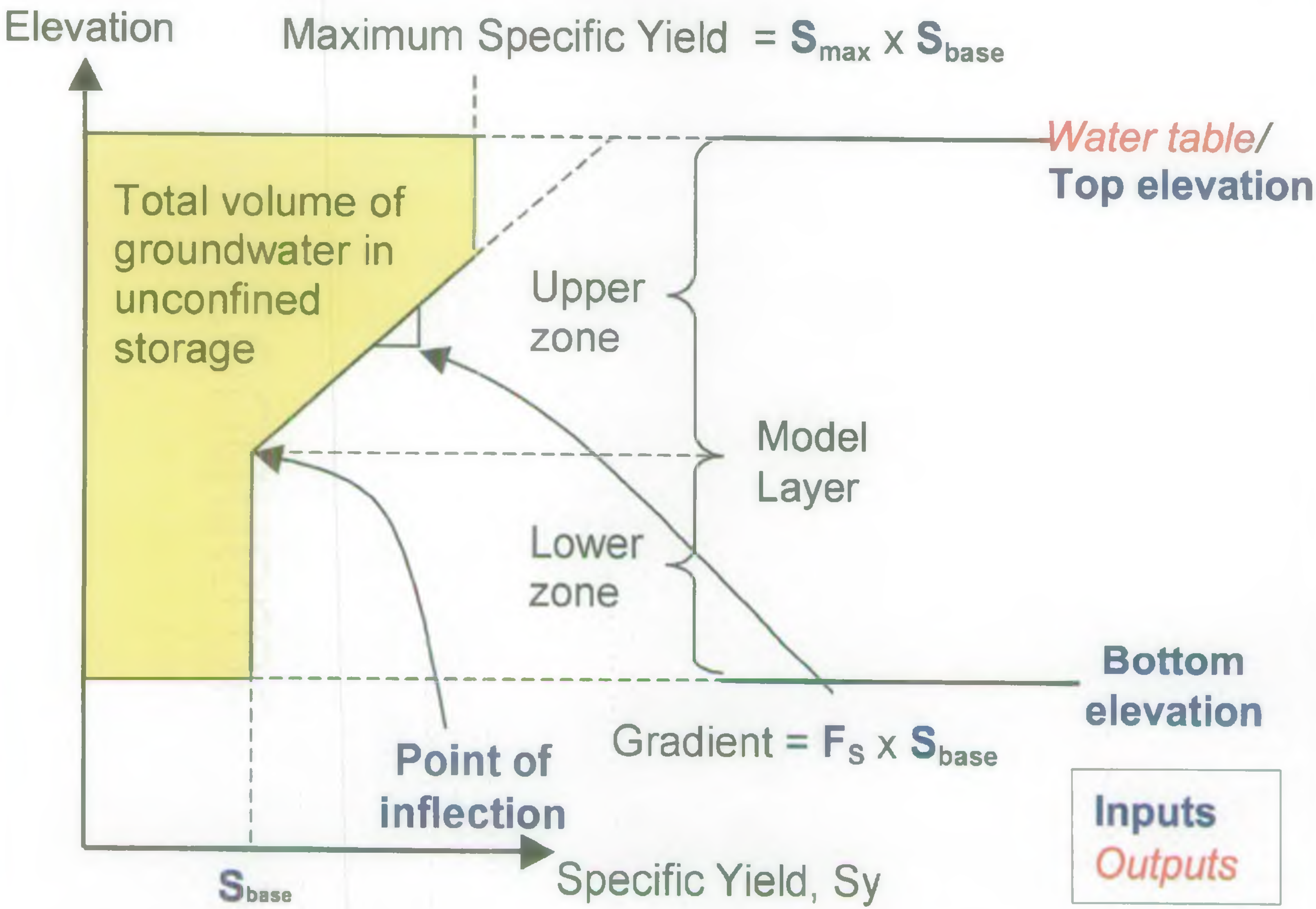


Figure 3.4 Conceptual model for the variation of hydraulic conductivity with depth

WATER MANAGEMENT CONSULTANTS

Figure 3.4



WATER MANAGEMENT CONSULTANTS

Figure 3.5 Conceptual model for the variation of storage with depth

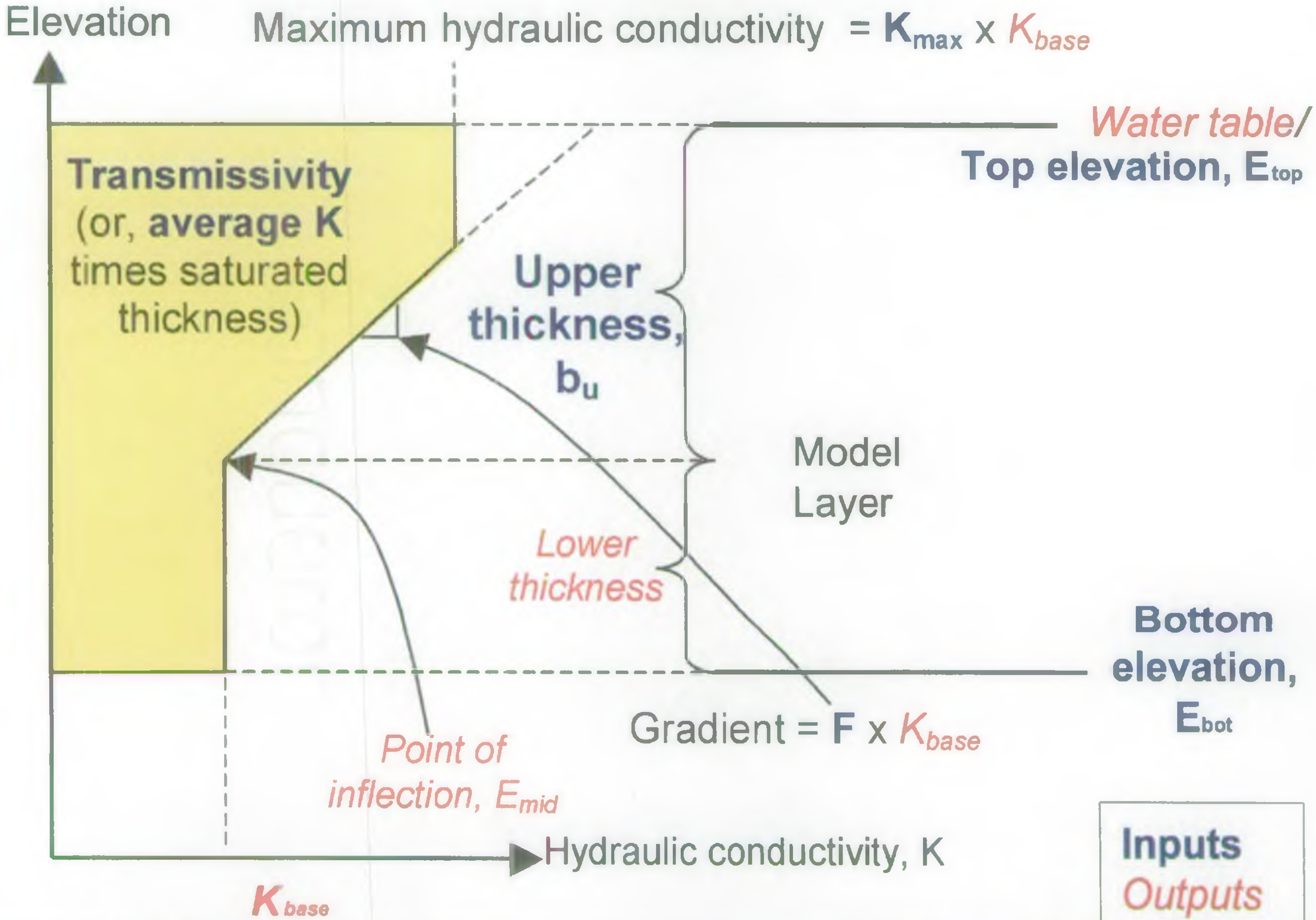


Figure 3.6 Inputs and outputs for automatic conversion option

4 TEST MODELS

4.1 Introduction

The code changes were tested using a variety of different models, including:

- Variations on the model used to test the code in Stage II of the project (Environment Agency, 1999).
- A new purpose-built three-layer test model.
- A model of the Itchen catchment under development by the Environment Agency Southern Region.
- A model of the Upper Lee catchment under development by Entec, consultants for Thames Region Environment Agency.

This section of the report first discusses some issues relating to setting up the initial conditions for a time variant run, and then discusses the results of the investigations using each of the models described above.

4.2 Approaches to modelling

4.2.1 Obtaining initial conditions for time-variant simulations

Time-instant steady-state (TISS)

Rushton & Redshaw (Rushton & Redshaw, 1979, Section 7.6) define the time taken to reach dynamic balance, starting from flat initial heads, as:

$$t = \frac{2.5L^2S}{T}$$

where:

t	=	time
L	=	length of a typical flow path in the aquifer
S	=	storage
T	=	transmissivity

For the Itchen model:
L ~ 10 km = 10,000 m,
S ~ 1% = 0.01
T ~ 800 m^2/d

therefore:
t ~ 3125 days = 8.6 years.

This is very sensitive to L, eg if L=5 km, t~2.1 years, suggesting that it takes longer to reach dynamic balance in areas distant from rivers.

However, Rushton & Redshaw's simulations started from flat initial heads, well below the heads when at dynamic balance; we are interested in starting from heads that are much closer to those at dynamic balance, so the times involved are generally shorter.

Practical approaches

When undertaking time-variant groundwater simulations it is important that the initial conditions used to start the simulation are realistic. Often, initial conditions are taken from the results of a steady-state simulation that represents average conditions in the aquifer. However, as groundwater conditions change with the seasons and respond to changes in abstraction, real aquifers are rarely in a condition that could be described as a 'steady state'.

The problem of initial conditions can be approached in several different ways. The first, most commonly used method is to run the model through several years, before the time period of interest, so that the model reaches 'dynamic balance'. A second, less commonly used method is to estimate the change in groundwater storage over the model over a time period of about a month, and add this to the recharge in a 'time-instant' steady state model.

Initial conditions become more of an issue when attempting to model an aquifer where hydraulic conductivity varies with depth. The problem is how to define a realistic hydraulic conductivity profile, when several different profiles can give the same transmissivity values, and hence the same steady state solution. *The effect of different hydraulic conductivity profiles on simulation results can only be assessed by looking at both high and low water table conditions.*

One way to estimate the way in which the hydraulic conductivity varies with depth is to obtain estimates of the transmissivity for high and low water table conditions, and then construct a hydraulic conductivity profile that gives the same high and low transmissivity values for the different water table levels.

The transmissivity values can be estimated in the normal ways (ie from observed groundwater gradients and flow estimates) and can be tested through model simulations. Environment Agency staff and consultants currently working with the code have suggested two main approaches, both involving construction of two models with fixed transmissivity values; one with low (autumn) transmissivities, the other with high (spring) transmissivities.

The approach suggested to simulate the Upper Lee catchment involves bypassing the steady state phase of the modelling, and instead undertaking two time variant simulations with different distributions of specified transmissivities. The time variant simulations start with some representative initial heads (ie contoured observed heads, or heads at surface elevation), and simulate a shortened historical sequence of recharge and abstraction. The first model has lower transmissivities, and is designed to reproduce the observed low flows over two or three years. The second model has higher transmissivities and is designed to reproduce high flows. The transmissivity distributions are then compared, and combined to derive the VKD parameters. The advantages of this approach are likely to be:

- The problems associated with steady state simulations are avoided.
- The effect of storage can be evaluated in the same simulations.

The disadvantages are likely to be:

- The effects of the storage coefficients on simulation results need to be differentiated from the effects of the VKD parameters through sensitivity analysis.
- It takes a relatively long time for the time-variant models to run and for any parameter changes to be assessed (compared to run times for steady state models).
- Care needs to taken to ensure that the model has reached dynamic balance.
- The method employed did not help pin down VKD parameters as there were too many other aspects of the modelling that were uncertain.

The second approach, proposed for modelling the River Bourne catchment, is to construct two time-instant steady state (TISS) models, one for maximum and one for minimum water table conditions. The strategy is to avoid the auto-conversion option available in the code (and hence avoid a "spotty" distribution of hydraulic conductivity with a different value in each cell) and use the same VKD parameters directly in each model. Selecting times of maximum and minimum groundwater heads (when there is little or no change in groundwater storage) avoids the difficulty in estimating the change in storage across the model. The advantages of this approach are likely to be:

- The ability of the model to reproduce maximum and minimum heads can be assessed before moving to a time variant model.
- The effect of the VKD parameters in conjunction with river coefficients can be evaluated independently of the storage coefficients.
- The run times of the steady state models should be quick compared to those of time-variant models (provided there are no convergence problems) allowing a wider variety of sensitivity runs to be carried out.
- The results of either of the steady state models could be used as stable initial conditions for a time-variant simulation.

The disadvantages of this approach are likely to be:

- There may be difficulties in getting the steady state models to converge without using the auto-conversion option (although the PCG2 solver in MODFLOW is more robust than the point SOR solver used in the Birmingham University code).
- The assumption of zero change in storage at maximum and minimum water table conditions may not be valid.

Both of these approaches avoid the use of the auto-conversion option, and allow the VKD parameters to be input directly (rather than the base hydraulic conductivity being calculated by the MODFLOW code, resulting in 'measles plots' of hydraulic conductivity). From the points discussed above it is not immediately clear which of the two approaches is more useful, but trials with operational models (Upper Lee and Bourne) are currently underway

4.3 Description of the test models

4.3.1 Modified Stage I & II models

The test model used to test the modifications carried out in Stage I of the project was a simple one layer model with inputs from areal recharge and discharge to a canal (represented by river cells). For this stage of the project, the model was modified to test the new modifications to the code. Aspects of the modifications which were tested using this model are summarised in Table 4.1.

Table 4.1 Summary of testing using variations on the Stage I model

Modification to code	Modification to model	Results of testing
Direct use of T_x and T_y values.	Specified transmissivity along rows (X-direction) set to zero in last column.	No change to model results.
Allow VKD in any layer (including confined VKD layers – LAYCON = 5).	Make model with two layers, with identical properties in each layer. Both layers unconfined (top of lower layer set above groundwater level).	Computed heads in both layers unchanged from previous versions of the model.
Include maximum hydraulic conductivity factor.	Added maximum hydraulic conductivity factor arrays with values high enough not to affect results.	Computed heads unchanged.
Automatically adjust upper thicknesses in auto-conversion if heads are too close to bottom elevation.	Set upper thicknesses to a value greater than the difference between the steady state heads and the bottom elevation.	Computed heads unchanged. Upper thicknesses automatically corrected, hydraulic conductivities changed.
Allow variable storage with depth (VSD).	Added VSD property arrays to time variant model.	Computed flows compared to those calculated in a spreadsheet from the computed heads and VSD properties. Total volumes agree to 0.0015%.

For a complete description of the various code changes and the modelling log, see Appendices A and B.

VSD was tested using variations on the test model used in Stage II of the MODFLOW-VKD project, and also on a three-layer test model (see following section). The results of the modified Stage II test model (unconfined) were verified using a spreadsheet that independently calculated the flows to and from storage based on the modelled groundwater heads and the storage parameters. A second variation of the Stage II test model was constructed with a layer top specified slightly above the steady-state groundwater heads so that confined conditions could be produced in the model. The results from this model were checked qualitatively (the heads rose sharply when they were above the top elevation and the lower, confined, storage coefficient came into effect), but a quantitative assessment was not made.

4.3.2 Multiple layer test model

In order to test the code changes with a fairly complex groundwater system a three layer test model was constructed with dipping layers (see Figure 4.1). The model included areal recharge, and discharge to a river and a stream. The geometry of the model was set up in such a way that the stream and the water table intersected successively lower layers further away from the river. This was intended to provide a numerically challenging problem for the modified code.

The model was initially set up with specified transmissivities (higher near the river and the stream), these layers were then converted to VKD layers using the auto-conversion routine.

This model proved to be useful in many ways, as it revealed many aspects of the model code and the general approach to modelling that needed to be addressed. For instance, the auto-conversion simulations resulted in changes being made to the way the code handled dry cells in the first part of the simulation, and to the correction of upper thicknesses should head values be too close to the bottom of the layer. Another problem that was highlighted by the auto-conversion simulations was that if the head calculated in a cell is very close to the bottom of the layer, the code calculates a very high value for the base hydraulic conductivity from the specified transmissivity. Partly for this reason, the code was later modified so that layers could be converted from constant hydraulic conductivity layers to VKD layers. This meant that if the saturated thickness of a cell was small, the corresponding transmissivity, and hence the calculated base hydraulic conductivity would also be smaller.

Testing of the new three-layer test model moved on to time-variant simulations using VSD. A recharge sequence was produced with one year of constant recharge at the steady-state rate, followed by three years of seasonal recharge. Despite using a large number of VSD parameter combinations and solver options, this model would not converge unless the maximum storage factor was set to one (constant specific yield with depth). To test whether the non-convergence of the model was due to the VSD parameters, the code modifications, or the general layout of the model (MODFLOW is known to have problems with certain multi-layer models), a variation of the model was constructed without variation of hydraulic conductivity or storage with depth. This model was run using both the modified code and an accepted Windows version of MODFLOW (MFWin32). The model failed to converge using both these versions of MODFLOW (in exactly the same place). From this two things were learned:

- The three-layer test model was too complex to be an effective tool for testing the modified code.
- The fact that the model converged with VKD and no VSD suggests that, rather than making the simulation unstable, VKD can make time variant simulations more stable. This is thought to be due to the reduction in the variability of groundwater heads, which is a consequence of utilising VKD in a numerical model.

Due to the problems with the three-layer test model, it was agreed that the further testing should be carried out using modifications to the Stage II test model (including multiple layer versions) and the Itchen and Mimram models. Further development of the three-layer test model was not continued.

4.3.3 Itchen model

Concurrently with this project a model of the Itchen catchment was being developed at the Environment Agency, Southern Region. As it is believed that variation of hydraulic properties with depth is an important feature of this catchment, it was thought to be a good opportunity to use the modified code in the development of the model.

Before introducing VKD into the Itchen model, an initial steady state model with constant hydraulic conductivity with depth (standard MODFLOW) was developed in-house at the Environment Agency. The parameters of this embryonic model were adjusted so as to reproduce the observed groundwater levels in the catchment.

The first task was to convert the model to include VKD. Zones were defined of different upper thickness and hydraulic conductivity gradient factors based on whether cells were in valleys close to rivers or on interfluves. An auto-conversion simulation was carried out which gave the base hydraulic conductivities at each cell. Because the calculation resulted in different values of base hydraulic conductivity at each cell, the next step was to lump these values into different zones. This was achieved by reducing the accuracy of the base hydraulic conductivities to two significant figures, resulting in 22 different zones. The simulation was then re-run, recycling the initial heads from runs with more zones and using relaxed convergence criteria. The effect of this zoning on the groundwater heads was minimal (+/- 0.2 m) throughout most of the model, but differences in head of 0.3 to 1.4 m were produced near pumping wells. This was considered unimportant, as further refinement of the model could reduce these differences if observations showed the levels to be incorrect.

The rivers in the Itchen model were originally represented using MODFLOW river cells. These were replaced by MODFLOW stream cells, which take into account flow routing down the river channels, enabling stretches of river to dry out and allowing accretion profiles to be plotted. Accretion profiles have been produced for all the rivers in the model. This change to the model made very little difference to the groundwater heads except around a small tributary of the River Itchen (segment 3). This segment is located above the groundwater heads in this area, but could not provide leakage (like the river had done) as there was no flow in the stream that could leak into the aquifer. If an inflow is added to the top of the segment, the results are identical to those from the model with river cells. If this tributary normally has flow in it then the stage of these stream cells should be checked, or the groundwater heads should be increased in order to produce this flow. However, it may be that the model is too coarse to accurately model heads and flows in such a small region of the model.

The changes to the stream routing package were tested using this model, and all the tests confirmed that the modified package was behaving as designed.

The time-instant steady-state (TISS) approach was investigated using the Itchen groundwater model. Three time-variant simulations were undertaken; the first started from long-term average steady-state (LTASS) conditions, the second from time-instant steady-state conditions from a dry month, and the third from TISS conditions from a wet month. The TISS conditions were calculated using the flows to and from storage produced by the first time variant model (the groundwater heads from this model could have been used instead, but the object was to investigate the TISS approach).

It should be pointed out that estimating the change in storage at each cell from field data (rather than using an existing model) would be more difficult. For this reason it is suggested that if this approach is used, that it be applied for times when groundwater levels are at a maximum or minimum, and changes in storage are minimal.

The total water balance for the three models was compared, along with the hydrographs from five different locations: northern interfluve, south-eastern low-K interfluve, beneath the northern and southern Tertiaries, and a river confluence. The water balance and hydrographs for the interfluves and confluence showed very little difference between the three models after one to two years. The hydrographs for the areas confined by the Tertiaries showed heads rising throughout the simulation by around 0.5 m in the north and falling by the same amount to the south. Due to these long-term changes beneath the low-K Tertiaries, the results of the three simulations were different in these areas by around 0.2 to 0.3 m. It was noted that the storage values specified for the areas confined by the Tertiaries were the same as for the unconfined chalk. This was an error, but it was not corrected at the time. The correction would mean that changes would propagate faster through this part of the model, which should reduce the differences between the simulation results.

The results of these investigations suggest that, for fast systems like the Itchen, the TISS approach is not required for reasons of numerical stability or accuracy even though the first year of a simulation is likely to be less accurate.

4.3.4 Upper Lee model

The Upper Lee model that was being developed by Entec was having some difficulty representing the heads and flows observed in the field. The flows in the model were too variable and the heads were not variable enough. VKD has the effect of making flows more variable and heads less variable. Therefore, this suggests that either the influence of the variation in hydraulic conductivity with depth was overemphasised in the model, the storage values were wrong, the time series of recharge was incorrect, or effects of delayed yield needed to be taken into account. As all these factors affect the time variant behaviour of the model, it is important that any equivalence between their effects be investigated using systematic and rigorous sensitivity analysis (Hill, 1998). In this case it could also be that the spatial distribution of recharge is wrong and is contributing to (but not the sole cause of) the problem. (Since the way Thames Region Environment Agency calculate their recharge is to have it all based on factors from a single rain gauge. Hence if it rains at that gauge it rains everywhere).

The modified stream routing package was also used with this model in conjunction with Entec's in-house recharge code.

WATER MANAGEMENT CONSULTANTS

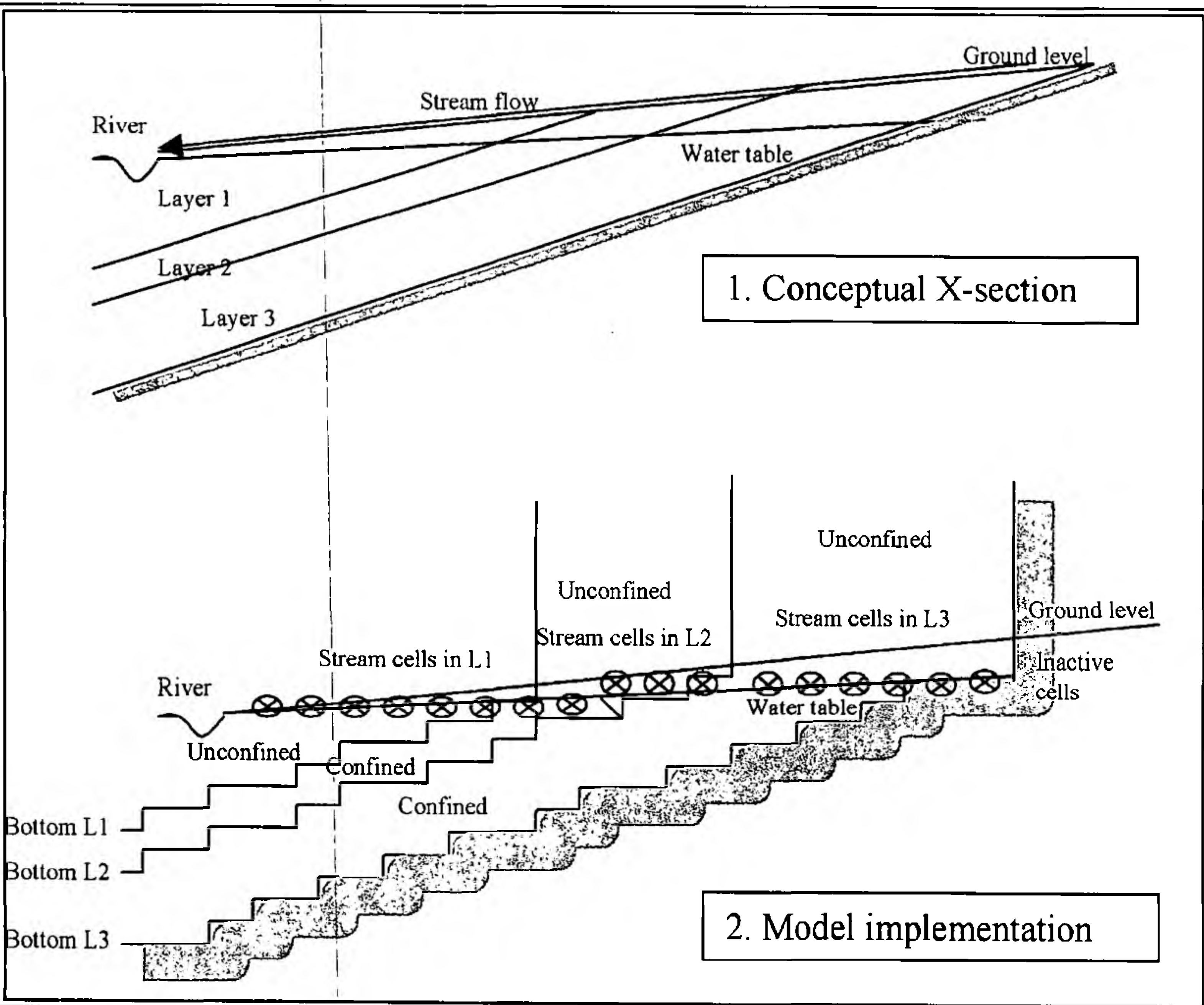


Figure 4.1 Schematic of three layer test model

5 SUMMARY, CONCLUSIONS AND RECOMMENDATIONS

5.1 Introduction

This section summarises the findings of the project, describes the uses and limitations of the modified MODFLOW code, and presents the conclusions and recommendations for further work. The following discussion is split into sub-sections relating to the modifications made to the code, limitations of the modified code, and the results of testing and modelling work.

5.2 Summary

5.2.1 Modifying the MODFLOW code

The original MODFLOW-96 code is well laid out and documented. The modular structure of the code not only makes it easy to add new packages (eg stream, reservoir or solver packages), but also means that the code is set out in a very logical way, with subroutines for each package having a clearly defined function. Comment lines throughout the code provide additional information on the function of each block of code.

The main areas of the code that have been investigated in this project are:

- The Block-Centred Flow module:
    - Use of the Layer-type codes
    - Transmissivity calculations
    - Storage calculations
    - Calculation of VKD parameters from standard MODFLOW simulations, including:
        - Handling of 'dry' cells in auto-conversion simulations
        - Control of array formats in BAS and BCF input files created by the code
        - Increased control of filenames for the second simulation.
- The Stream Routing module:
    - Use of specified discharges or abstractions at any stream node
    - Stream routing – connection of tributary flows to any stream node
    - Calculation and output of flow budget terms

- The Preconditioned Conjugate-Gradient solver module (PCG2):
    - Convergence criteria
    - Run time output of maximum head change and residual
    - Checking convergence criteria over multiple outer iterations
    - Output of heads calculated during iterations for debugging purposes.
- The Utilities module:
    - Use of 'direct access' binary files for compatibility with Groundwater Vistas.

All the modifications have been highlighted in the code, and the original code commented out for comparison. Additional comment lines have been inserted where necessary.

5.2.2 Application of the modified MODFLOW code

The modified MODFLOW code has been designed to simulate groundwater flow in formations where hydraulic parameters vary with depth, as observed in fissured systems such as chalk and limestone aquifers. The modifications allow both hydraulic conductivity and specific yield to reduce gradually with depth within any individual model layer. This allows models to simulate groundwater flow behaviour that would otherwise require a complex multi-layer model (which is likely to suffer from problems with de-saturation and re-saturation of model cells).

The code can also be used to convert existing MODFLOW models to models with VKD, by setting a flag and adding some property arrays in the BCF input file. In this way it is possible to create VKD models that produce identical steady state results to the original model, but which behave differently in response to seasonal patterns of recharge and abstraction.

The modifications to the stream module allow greater control of abstractions, discharges and connections to tributaries. This also means that the runoff component of the stream flow can be added at each individual node.

5.2.3 Limitations

The modified code has the following known limitations:

- Hydraulic conductivity and specific yield can only decrease with depth within a single model layer. Increases in hydraulic properties with depth would have to be represented by additional layers.
- Other effects associated with chalk aquifers, such as dual porosity and delayed yield, have not been included.
- In some cases the non-linearity of the transmissivity profile may make it difficult for the solvers to find a solution to steady state problems unless the starting heads are very close to the correct solution (as they are when using the auto-conversion option). This is not always the case however, and for time-variant runs VKD actually appears to make it easier for the solvers to converge on a solution.

- Specifying VSD in a time-variant model can often result in numerical instabilities and non-convergence (see Section 3.3.2), especially if conditions are changing between confined and unconfined. If this is thought to be an important feature of the catchment of interest, and problems are encountered, it is recommended that the change in storage is represented as a near step function; with a high value for the gradient factor and a realistic maximum factor. Solver parameters (such as damping factors) should also be investigated.

- The auto-conversion option produces unique base hydraulic conductivity values for each model cell with VKD, without any kind of grouping into zones. Zoning can be carried out manually, and it is recommended that the values are checked to make sure that they are realistic.

- When specifying surface water abstractions for streams, the actual amount that can be abstracted is limited by the flow available in that stream reach. If the abstraction rate is reduced a message is written to the output file.

- At present, particle tracking codes such as MODPATH or transport codes such as MT3D cannot be used with MODFLOW-VKD as these codes assume that flow is evenly distributed over the entire depth of each model cell, which is not the case in cells where VKD is active.

5.2.4 Approach to modelling and testing of the modified code

To test the modifications to the MODFLOW code a number of different models were used. Some of the models were purpose-built test models, originally simple, to which complexity was gradually added to test different aspects of the code modifications. In addition, working regional models developed by the Agency were also used; one of the Itchen catchment (Southern Region), and the other of the Upper Lee catchment (Thames Region). These models were used to test different approaches to using the VKD capability for modelling real chalk groundwater systems, to test that the modifications were working correctly, and highlight any problems or capabilities that needed to be added to the code during development.

5.3 Conclusions

The following capabilities have been successfully implemented in the MODFLOW-VKD code:

- Variation of hydraulic conductivity with depth (VKD) in any model layer (including layers that can become confined).

- Variation of specific yield with depth (VSD) in any model layer (including layers that can become confined).

- Changes to the auto-conversion routine (which converts normal MODFLOW layers to VKD layers) to take account of the changes above.

In the course of the project some additional code changes were also requested and incorporated into the code. These were:

- A maximum hydraulic conductivity and specific yield factor for each model cell where VKD is active.
- Modifications to the stream routing package to allow discharges, abstractions or tributary inflows to be specified at any stream node.
- An output of model progress to the screen when using the PCG solver package.
- Option to allow binary output files to be created in the same format as those required by Groundwater Vistas (GV – Environmental Simulations Inc, 2001), the Agency's preferred MODFLOW user interface.
- Option to allow the input of X- and Y-direction transmissivities or hydraulic conductivities independently (without using the anisotropy ratio method).
- Option to allow convergence to be forced if the convergence criteria are met for a specified number of outer iterations (this was not thought to be a particularly useful option, but was included to make the code compatible with models produced by GV).
- A debugging option for the PCG solver so that the evolution of head values at each iteration could be examined – to identify problem areas in models that do not converge.

These changes to the code were then tested to ensure that the code behaved correctly. This testing was undertaken both with test models and operational models representing real case studies. Testing the code in the development of operational models revealed issues that are likely to be encountered in the future, and allowed these issues to be addressed.

The end product of this stage of the project is a fully functioning, backward compatible version of MODFLOW which allows for vertical variation of hydraulic conductivity and specific yield in any layer of a groundwater model.

5.4 Recommendations for future work

The work undertaken in this project has shown that the MODFLOW code can be successfully modified to more accurately represent flow processes important in UK hydrogeology, provided that care is taken to think through the modifications beforehand, and that the code is then thoroughly benchmarked and tested.

Possible directions for further work related to this project are outlined below:

- Further investigation into methods of estimating how hydraulic properties vary with depth in real chalk and limestone systems, and how to translate the findings into groundwater flow models.

- Comparison of the MODFLOW-VKD code with the new Hydrogeologic-Unit Flow (HUF) package available with MODFLOW-2000 (Anderman & Hill, 2000). The HUF package also allows hydraulic conductivity and specific yield to vary within a model layer, but works in a different way to the VKD code.

- Further investigation of the instabilities encountered when variations in storage are specified, and ways to combat these instabilities.

- Consideration of other important issues in chalk and limestone hydrology, such as dual porosity, delayed yield, and the various effects of fissure flow on mass transport.

- Investigate alternative ways of handling the drying and rewetting of cells in MODFLOW, such as allowing a small residual transmissivity in each cell so that all cells remain active. The authors are aware that personnel at the USGS (along with other independent organisations and individuals) are also interested in this line of research (Doherty, 2001).

REFERENCES

Allen, D J, Brewerton, L J, Coleby, L M, Gibbs, B R, Lewis, M A, MacDonald, A M, Wagstaff, S J, Williams, A T, 1997. *The physical properties of major aquifers in England and Wales.* British Geological Survey Technical Report WD/97/34.

Cross, G A, Rushton, K R, Tomlinson, L M, 1995. *The East Kent Chalk Aquifer during the 1988-92 drought.* Journal of the Institution of Water and Environmental Management, 9, pp. 37-48.

Doherty, J, 2001. *Improved Calculations for Dewatered Cells.* Groundwater, Vol. 39, No.6 - Nov-Dec 2001, p 863.

Environment Agency, 2002. *User Guide for MODFLOW-VKD – A Modified Version Of MODFLOW-96 to Include Variations in Hydraulic Properties with Depth.* Environment Agency. ISBN: 1 857 05766 X.

Environment Agency, 2001. *Bourne and Nine Mile Rivers low flow investigation, conceptual modelling report.*

Environment Agency, 2000. *MODFLOW-VKD Stage III Report: Investigation using Southwest Chilterns Model.* Environment Agency. ISBN: 1 857 05360 5.

Environment Agency, 1999. *Representation of the variation of hydraulic conductivity with saturated thickness in MODFLOW. Stages I & II. Code changes and testing against Birmingham University code.* Environment Agency. ISBN: 0 857 05194 7.

Environmental Simulations Inc, 2001. *Guide to Using Groundwater Vistas*, Rendon, Virginia, USA.

Foster, S S D, Milton, V A, 1974. *The permeability and storage of an unconfined chalk aquifer.* Hydrological Sciences – Bulletin – des Sciences Hydrologiques, XIX, 4, pp. 485-499.

Harbaugh, A W, McDonald, M G, 1996, *User's documentation for the U.S. Geological Survey modular finite-difference ground-water flow model*: U.S. Geological Survey Open-File Report 96-485.

Headworth, H G, Keating, T, Packman M J, 1982. *Evidence for a shallow, highly permeable zone in the Chalk of Hampshire.* Journal of Hydrology, 55, 93-112.

Hill, M C, 1998. *Methods and Guidelines for Effective Model Calibration.* U.S. Geological Survey Water-Resources Investigations Report 98-4005.

Hill, M C, 1990. Preconditioned Conjugate-Gradient 2 (PCG2*), A computer program for solving ground-water flow equations.* U.S. Geological Survey.

Kladias, M P, Ruskauff, G J, 1996. *Computer note on implementing spatially variable anisotropy in MODFLOW.* Geraghty and Miller, Inc and INTERA, Inc.

McDonald, M G, Harbaugh, A W, 1988. *A modular three-dimensional finite-difference ground-water flow model.* U.S. Geological Survey, Techniques of Water Resources Investigations. Book 6, Chapter A1.

Owen, M, 1981. The Thames groundwater scheme. *In Case-Studies in Groundwater Resources Evaluation*, J.W. Lloyd (editor), pp. 186-202. Clarendon Press, Oxford.

Price, M, Downing, R A, Edmunds, W M, 1993. *The Chalk as an aquifer. 35-58 in The hydrogeology of the Chalk of north-west Europe*, Downing, R A, Price, M., Jones, G P (editors). Clarendon Press, Oxford.

Price M, Low R and McCann C, 2000. *Mechanisms of water storage and flow in the unsaturated zone of the Chalk aquifer.* Journal of Hydrology. Vol 233, p 54-71.

Prudic, D E, 1989. *Documentation of a computer program to simulate stream-aquifer relations using a modular, finite-difference, ground-water flow model.* U.S. Geological Survey.

Robinson, V K, 1975. *Ground Water Development Scheme, Report on Borehole Geophysical Logging Carried out During Stage I.* Thames Water. IR58.

Rushton, K R, Chan Y K, 1976. *Pumping test analysis when parameters vary with depth. Ground Water.* 14, 82-87.

Rushton, K R, Connorton, B J, Tomlinson, L M, 1989. *Estimation of the groundwater resources of the Berkshire Downs supported by mathematical modelling.* Quarterly Journal of Engineering Geology, London, Vol. 22, pp. 329-341.

Rushton, K R, Fawthrop, N P, 1991. *Groundwater support of stream flows in Cambridge area, UK. Hydrological Basis of Ecologically Sound Management of Soil and Groundwater.* IAHS Publication No. 202, 367-376.

Rushton, K R, Rathod, K S, 1980. *Aquifer response due to zones of higher permeability and storage coefficient.* Journal of Hydrology, 50, 299-316.

Rushton, K R, & Redshaw, S C, 1979. *Seepage and Groundwater Flow.* John Wiley & Sons, Ltd.

Rushton, K R, Smith, E J, Tomlinson, L M, 1982.*An improved understanding of flow in a limestone aquifer using field evidence and mathematical models.* Journal of the Institution of Water Engineers and Scientists, Vol. 36, pp. 369 -387.

WS Atkins Consultants Ltd., July 2001. *Upper Lee Groundwater Model. Borehole geophysical log interpretation for verification of VKD.*

APPENDIX A
Code changes

CODE CHANGES – SUMMARY TABLE

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
1. Spatially variable anisotropy Executable: 'mfwvk1.exe' Modules: 'modflw96.f01' 'bcf5.f01' (based on 'modflw96.for' & 'bcf5.for')	Changes based on those described by Ruskauff & Kladias in 'Computer Note On Implementing Spatially Variable Anisotropy In Modflow'. Change code to read flag which indicates whether node by node anisotropy is required (ITRPY (=1) - Read in format I10 from first line of *.BCF file, after IHDWET) Add ITRPY to end of the list of variables passed between subroutines which use TRPY array ('call' and 'subroutine' statements in both 'modflw96.f01' and 'bcf5.f01') Increase size of TRPY-array from 1-d (layers) to 3-d (nodes), allocate space in the X-array (even if ITRPY=0) and change dimension statements at start of each subroutine Change code to read TRPY array into either all (ITRPY=1) or part (ITRPY=0) of the space allocated for it, using subroutine U2DREL (instead of U1DREL) Change code in the conductance calculation subroutines (SBCF5C, SBCF5A, SBCF5L and SBCF5U) to calculate the conductances using variable anisotropy (if ITRPY=1)	Insert flag value of 1 (or greater) into 80th column of first row of *.BCF package (ITRPY; after IHDWET) Replace 1-d anisotropy input line { TRPY (NLAY) } with standard 2-d (real) formatted input { TRPY (NCOL, NROW, NLAY) }. Arrays for all layers should be input sequentially, before the lines that specify DELR and DELC.	Ran 'SpecT1' (Nodal Trans). Results compared with those from using 'MFWin32' – identical. Results compared with those from KRs model - similar (132 head values (out 525) out by 0.1 meters) ...(should also try with existing more complicated anisotropic model (Tadcaster?) and compare with MFWin32 – try using all 4 LACON and LAYAVG values)... Ran 'SpecT1u' (unconfined version of SpecT1) for comparison with MFWin32 (Identical) and SpecT2u (not identical - see next stage)

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
2. Internodal transmissivity / hydraulic conductivity. Executable: 'mfwvk2.exe' Module: 'bcf5.f02' (based on 'bcf5.fo1')	Change code to allow values of LAYAVG up to 40 (previously 30) Add fifth character string to AVGNAM array: 'INTERNODAL ' For constant Transmissivity simulations: set initial values of CR array (conductance along rows) equal to CC array (conductance along columns) equal to x-direction transmissivity (CC array is later multiplied by the anisotropy (TRPY) to give the y-direction transmissivity) Change code which calculates saturated thickness for unconfined simulations: Previously the saturated thickness was calculated at each node and the modeller specified an averaging system (via LAYAVG) to calculate the internodal conductance Now, if hydraulic conductivity is specified between nodes, the saturated thickness is calculated from the (arithmetic) average of the heads and the bottom elevations at the two relevant nodes (therefore, two different saturated thicknesses are calculated: one for the x-direction and one for the y). . Calculated transmissivities are stored in the CC and CR arrays before being passed to the new subroutine to calculate conductances New subroutine added to calculate internodal conductances using internodal Trans / hyd-cond: Based on the old 'arithmetic averaging' subroutine, the new subroutine takes values of internodal transmissivity (in the CC and CR arrays) and converts them to conductances using the cell dimensions (DELC and DELR) and the anisotropy ratio (TRPY). Change code so that, if cells become dry, not only CC but CR also is set to zero.	Type '4' into 1st column of 2nd row of the *.BCF package (just before LAYCON number) this sets LAYAVG=40 and AVGNAM=4 - Internodal transmissivity / hydraulic conductivity Put internodal values of transmissivity or hydraulic conductivity (X-direction) into the relevant input array (values input are applied to the right hand face of the cell) Put internodal values of anisotropy (if ITRPY=1) into relevant array - this gives the multipier to be applied to the x-direction Trans / hyd-cond to give a y-direction trans / hyd-cond (applied to the front face of the cell)	Ran 'SpecT2' (Internodal Trans) and results compared with those from 'SpecT1' using 'mfwvk1.exe' - Identical Ran 'SpecT2a' (with no-flow cell in centre) - realistic results Ran 'SpecT2b' (with very high T values in last (unused) column) - identical to 'SpecT2' Ran 'SpecT2c' (reproducing erroneous Ts in column 14 of KRs model) - improved match with results (9 values out by 0.1 meters) Ran 'SpecT2u' (unconfined version of SpecT2) for comparison with SpecT1u - results similar but not identical as 'mfwvk1.exe' calculates two transmissivities seperately and averages them; whereas 'mfwvk2.exe' averages two thicknesses and then calculates the transmissivity.

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
3. Internodal top and bottom elevations Executable: N/A… Module: 'bcf5.f03' (based on 'bcf5.fo2') ABANDONED – CODE CHANGES NOT REQUIRED	Change code to allow values of LAYAVG up to 50 Add sixth character string to AVGNAM array: 'INTER ELEV ' Increase size of TOP and BOT arrays to allow internodal input Every time top and bottom arrays are called (i.e. for dry cell or confined / unconfined conversions) code has been changed to make sure the correct array is being used (as two TOP and BOT arrays are needed if internodal elevations are to be specified) Change code to use average value of internodal elevations for node centered calculations such as dry cell and confined / unconfined conversions Use internodal top and bottom elevations to calculate internodal transmissivities if layer is unconfined. …ABANDONED – CODE CHANGES NOT REQUIRED	Type '5' into 1st column of 2nd row of the *.BCF package (just before LAYCON number) this sets LAYAVG=50 and AVGNAM=5 - Internodal transmissivity / hydraulic conductivity, top and bottom elevations Put internodal values of top and bottom elevations (X-direction then Y-direction) into the relevant input arrays (values input are applied to the right and front faces of the cell respectively)	N/A… ABANDONED – CODE CHANGES NOT REQUIRED
4. Variable hydraulic conductivity with depth (VKD) Executable: 'mfwvk3.exe' Modules: 'bcf5.f04' 'modflw96.f02' (based on 'bcf5.f02'& 'modflw96.f01')	Change code to allow values of LAYCON up to 4 Allocate space in the X-array for the VKGRAD array Add new ANAME label (in BCF5RP): ' HYDRAULIC COND GRADIENT' Read in VKGRAD array after TOP array (using U2DREL) Add VKGRAD to end of the list of variables passed between subroutines which use VKGRAD array ('call' and 'subroutine' statements in both 'modflw96.f02' and 'bcf5.f04') Change all 'if' statements involving 'LAYCON' to include option for LAYCON=4 (i.e. for establishing whether top and bottom arrays are used – LAYCON=4, same as LAYCON=3; both TOP and BOT arrays used) (note: this involves a lot of changes within the code, to avoid this it would be possible to modify the code to use a different flag for VKD and set LAYCON=3) Add 'if' statements (LAYCON=4) and counter (KG) to determine whether hydraulic conductivity gradients (VKGRAD) are to be used for a layer. Change calculation for transmissivity in SBCF5H, using the heads from the last timestep to calculate saturated thickness.	Type '4' into 2nd column of 2nd row of the *.BCF package (LAYCON number) this activates the VKD mechanism Uses same inputs as LAYCON=3 (HY, TOP, BOT, SC1, SC2) plus array for the hydraulic conductivity gradient factor (VKGRAD), entered after the TOP elevation array. Initial heads (in the *.BAS package) should be those calculated in the specified transmissivity model (as the transmissivity calculation uses the heads from the previous timestep).	Ran 'VKD1' (with hydraulic conductivities and top and bottom elevations from KRs input tables) – results compare well with KRs model, 'SpecT1' and 'SpecT2'. Ran 'VKD2' (with uniform initial heads) results were very wrong – see modelling log for details

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
5. Output format changed Executable: 'mfwvk3' Module: 'utl5.f01' (based on 'utl5.for')	Increase maximum length of output line (in sub UCOLNO) from 130 to 300 characters (BF array, check for NTOT, do loop (20) and format statement (31)) Increase maximum number of values in a row from 10 to 30 (in sub ULAPRW, for IP=12) Change allows easier examination of input & results	Set IPRN for relevant input array (e.g. hydraulic conductivity) equal to 0 or 12.	Incorporated into 'mfwvk3'. Improves layout of *.LST file for this particular model. Will be incorporated into all versions of MODFLOW for this study.
6. Automatic change from Specified transmissivity to VKD model (for initial steady state run) Executable: 'mfwvk4' Modules: 'bcf5.f05' 'modflw96.f03' (based on 'bcf5.f04' & 'modflw96.f02')	At end of loop to read layer information in BCF5RP, if ISS=2 & LAYCON(K)=4 then call subroutine SBCF5V Add subroutine SBCF5V. This sets transmissivity (CC) array equal to values read into the hydraulic conductivity array (HY), ignores the top and bottom arrays input for this layer by reducing the top and bottom location counters (KB & KT), and sets LAYCON=0 (Confined – specified T) for the layer. At end of simulation in MAIN ('modflw96.f03'), if ISS=2 call subroutine BCF5VK. Subroutine BCF5VK added. Reads old 'name file' and produces new one with new filenames for output files and BAS & BCF packages Reads old BAS package, writes new one (under a different name – BA2) with final heads from specified T model set as initial heads Reads old BCF package, uses calculated heads, transmissivity, hydraulic conductivity gradient factor and top & bottom thicknesses to calculate & output (to BC2) hyd-cond and top & bottom elevations, sets LAYCON=4 and ISS=1 Add subroutine B12DRI (based on U2DINT) Reads one or two dimensional 'real' arrays Allows output in same format as input (Was also intended to read integer arrays (i.e. IBOUND) but problems were encountered from converting from real to integer values) Return to start of MAIN using new 'name file' to give input instructions for steady state VKD run	Set ISS (steady state flag – first number in BCF package) = 2 Input arrays for transmissivity, thickness of botton zone, thickness of top zone, and hydraulic conductivity gradient factor for layer 1 New input files are automatically created with filenames based on the original input filenames but with the last character changed to a '2' (e.g. *.NA2, *.BA2 & *.BC2	Ran 'VKD3' with transmssivities, VKGRAD, and top & bottom thicknesses from KR's model: Values of calculated head consistent with previous runs Need input format for new BAS & BCF packages to have enough significant figures to accurately reproduce transmissivities

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
7. Allow printouts of internodal transmissivity values calculated at end of each timestep. Executable: 'mfwvk5' Modules: 'bcf5.f06' 'modflw96.f04' (based on 'bcf5.f05' & 'modflw96.f03')	At end of timestep calculation in MAIN ('modflw96.f04'), just before heads are printed or saved, call subroutine BCF5OT Add subroutine BCF5OT to end of BCF package: Calculate internodal transmissivities from 'branch conductances' (arrays CC & CR) and print in output file.	No changes to input files – transmissivity output is automatic at present	Ran 'VKD3' and 'VKD1' to check values of transmissivity used. Values OK if input arrays in BCF package are specified to sufficient significant figures
8. Correct small error in code which allows automatic change from SpecT to VKD to work with either Lahey or Salford compilers Executable: 'mfwvk6' Modules: 'moflw96.f05' (based on 'modflw96.f04')	Close all files (except listing output file) before reopening *.NAM, *.BAS & *.BCF files and writing new files.	No change	Tested using Lahey and Salford compilers – both work and give same results.

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
9. Introduce input flag to determine whether transmissivty is based on heads from last timestep. Executable: 'mfwvk7' Modules: 'bcf5.f07' 'modflw96.f06' (based on 'bcf5.f06' & 'modflw96.f05')	Change code to read flag which indicates whether transmissivity should be based on head from last timestep (IHOLD (=1) - Read in format I10 from first line of *.BCF file, after ITRPY) Add IHOLD to end of the list of variables passed between subroutines BCF5AL, BCF5FM & SBCF5H ('call' and 'subroutine' statements in both 'modflw96.f06' and 'bcf5.f07') Change code in the transmissivity calculation subroutine (SBCF5H) to check if IHOLD=1. If it does, use head from last timestep (HOLD). (Previously the code checked to see if LAYCON=4 before using the head from the last timestep.) (If IHOLD is not 1, transmissivity is updated every iteration) Also change subroutine BCF5VK to include IHOLD (both for reading of old BCF file and writing of new BC2 file)	Insert flag value of 1 into 90th column of first row of *.BCF package (IHOLD; after ITRPY)	Ran 'VKD5' (automatic SpecT to VKD, with stream) with IHOLD=0. Very small differences to 2nd part of output (less than 0.1% change in transmssivity, one value of head changed by 0.1 m, <0.01% change in global water balance) Ran 'VKD2a' (simple VKD problem with flat initial heads) with IHOLD=0. Model failed to converge which is better than producing erroneous results as it did when using initial heads to set transmissivity. Ran 'VKD2b' (with approximate head distribution for initial conditions) with IHOLD=0. Model converged and produced accurate results. Ran 'VKD6-tv4a' (identical to 'VKD6-tv4' but as IHOLD is effectively zero, transmissivity is updated every iteration). Results very similar to 'VKD6-tv4' but more iterations needed to reach solution.

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
10. Allow input of Tx & Ty or Kx and Ky instead of the anisotropy ratio. Executable: 'mfwvk8' Modules: 'bcf5.f08' (based on 'bcf5.f07')	Change code to not read in TRPY array in normal way if ITRPY=2 Change to read second (Y-direction) transmissivity (or hydraulic conductivity) array into TRPY array. Divide TRPY array by first (X-direction) transmissivity (or hyd. cond.) array. Add extra titles to ANAME array for output to listing file (including titles used in automatic SpecT to VKD conversion – overlooked previously) Do same for subroutine BCF5VK (both for reading of old BCF file and writing of new BC2 file)	Insert flag value of 2 into 80th column of first row of *.BCF package (ITRPY; after IHDWET) Leave out TRPY array (i.e. put column spacings directly after LAYCON values) Add array of Ty (or Ky) directly after Tx (or Kx)	Ran 'VKD5b' (using TRPY=2 option). Very small differences from 'VKD5' (~0.01%).
11. Reproduce KR's error in the calculation of Ky. Executable: 'mfwvk9' Modules: 'bcf5.f09' (based on 'bcf5.f08')	Change code to use thickness of top zone averaged between a cell and the next one in the x-direction (rather than the next one in the y-direction) for calculation of the hydraulic conductivity when the automatic specified T to VKD option is used (ISS=2).	No changes required	Ran 'VKD3b' (using TRPY=2 option). Ky values quoted in KR's original document are reproduced. NOT USED IN SUBSEQUENT VERSIONS.
12. Allow a stream inflow to specified at any reach. Executable: 'mfwvk10' Modules: 'str1.f01' (based on 'str1.for')	Change code to put user specified inflow into a cell whatever reach number it has (not just the first reach). Make change to then add outflow from upstream reach to inflow of current one (not just set it equal to the upstream outflow). (Note: also uses 'bcf5.f08' rather than 'bcf5.f09')	Put a value into the column reserved for stream inflow (previously this number was ignored for all but the first reach in a stream segment).	Ran 'VKD6-tv5' and 'VKD6-tv5b'. Results compared well with KR's model (except for negative flows in stream).

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
13. Reproduce KR's error in the calculation of accumulated stream flow. Executable: 'mfwvk11' Modules: 'str1.f02' (also uses 'bcf5.f08' rather than 'bcf5.f09') (based on 'str1.f01')	Allow leakage from a reach to exceed the inflow into the reach.	No changes to input files	Ran 'VKD6-tv5a', results compare well with KR's results. All heads within 0.5% of KR's heads. Global flow balance within 0.5% of KR's values (except in month 8 of year 2 ~ 0.55%). Stream & river flows within 2% of KR's total accumulatec flow. Transmissivity mostly within 1% of KR's values (exceptions occur at the interfluves during the constant recharge year ~ 1.4%, and at the end of the simulation ~ 2.6%)
14. Correct transmissivity calculation to use average VKGRAD when internodal Ks are used Executable: 'mfwvk12' Modules: 'bcf5.f10' (based on 'bcf5.f08')	Corrected to use average of two VKGRAD values when calculating internodal transmissivities with VKD (subroutine SBCF5H).	No changes	Reran 'VKD6-tv5b' – output file identical to that created by using 'mfwvk10' (VKGRAD values are the same all over the model).

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
15. Change to always use implicit formulation for Transmissivity calculation when running a steady state simulation Executable: 'mfwvk13' Modules: 'bcf5.f11' (based on 'bcf5.f10')	Change to always use implicit formulation for Transmissivity calculation when running a steady state simulation (ISS is not 0) whatever value of IHOLD is entered. pass ISS flag to subroutine SBCF5H	no changes (don't need to be so careful when specifying IHOLD when running a steady state model).	Ran 'VKD6-tv5b' – no change to output file Ran 'VKD3c' twice – once with IHOLD=0, then with IHOLD=1 – no change to output files in either case.
16. Change to allow the top elevation to be equal to the bottom elevation for VKD simulations. Executable: 'mfwvk14' Modules: 'bcf5.f12' (based on 'bcf5.f11')	Change calculation of saturated thickness at each face (internodal option – LAYAVG=40) to always use the head rather than the top elevation. The saturated thickness is not used directly to calculate the transmissivity (when LAYAVG=40) but is used to tell when a cell becomes dry. Add line to calculate saturated thickness at a cell (LAYAGV is not 40) using the head (and not the top elevation) if VKD is being used (LAYCON=4).	No changes to data files (but allows the top elevation to be set equal to the bottom elevation without cells going dry when using the VKD option – for modelling an aquifer without a constant K zone).	Ran 'VKD5c' (with zero bottom thickness) – converged ok – no dry cells produced.

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
17. Change to allow dry cells when using internodal hydraulic conductivity. Executable: 'mfwvk15' Modules: 'bcf5.f13' (based on 'bcf5.f12')	Having tested the code under a situation where dry cells arise (bottom elevations above steady state heads) it was found that more than one cell needed to have the head below the bottom (in order to make the internodal thicknesses less than zero) and that if one cell did become dry, many others would also become dry without good reason. Change to calculate thickness at a node to see whether or not it should become dry (rather than at each cell face). Only calculate an internodal transmissivity if both the two cells are active.	No changes	Ran 'VKD6b' and 'VKD6c' (both with raised bottom and top elevations in the centre of the model) – both converged producing sensible results.
18. Change to use the same input formats for created input files when using the automatic SpecT to VKD option. Executable: 'mfwvk16' Modules: 'bcf5.f14' (based on 'bcf5.f13')	Change subroutines 'BCF5VK' and 'B12DRI' to read and reuse the original format statements in the '*.BAS' and '*.BCF' input files (for all the 'real' arrays – not for the integer IBOUND array). Add the format string to the arguments for subroutine 'B12DRI' (which reads the input arrays) Put these format strings into an array which is used when the new input files are written.	Change input formats in the '*.BAS' and '*.BCF' files to match the formats required in the new '*.BA2' and '*.BC2' files created by MODFLOW.	Tested using 'VKD5d' (with different input formats for each array) – formats accurately reproduced (will still reproduce entire array of identical numbers rather than a single value if all values in an array are identical).

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
19. Change to reset titles printed to output file to the original ones when using the SpecT to VKD option. Executable: 'mfwvk17' Modules: 'bcf5.f15' (based on 'bcf5.f14')	Add an 'else block' to the 'if block' which changes the titles when the SpecT -> VKD option is specified (ISS=2). The else block changes the titles back to the original titles when running the second part of a SpecT -> VKD model.	No changes	Tested using 'VKD5d' – titles in the 2nd output file are now corrected. (they now read: "HYD. COND.', 'BOTTOM' & 'TOP' rather than 'TRANSMISSIVITY', 'THICKNESS OF UPPER ZONE' & 'THICKNESS OF LOWER ZONE').
20. Introduce flag to activate the output of internodal transmissivities to the listing file. Executable: 'mfwvk18' Modules: 'bcf5.f16' 'modflw96.f07' (based on 'bcf5.f15' and 'modflw96.f06')	Change code to read flag which indicates whether transmissivity should be printed to the listing file every timestep (ITRANS (=1) - Read in format I10 from first line of *.BCF file, after IHOLD) Add ITRANS to end of the list of variables passed between subroutine BCF5AL ('call' statement in 'modflw96.f07' and 'subroutine' statement in 'bcf5.f16') Add 'if' statement (checking value of ITRANS) to line in 'modflw96.f07' which calls subroutine BCF5OT (which prints transmissivities to listing file).	Insert a non zero integer into 100th column of first row of *.BCF package (ITRANS; after IHOLD)	Tested using 'VKD6-tv5' – both with ITRANS = 1 and ITRANS = 0. No change to listing file for ITRANS = 1, for ITRANS = 0, no transmissivities are output to the listing file.
21. Allow the header	Correct the code in subroutine BCF5VK to write the	No changes	Tested using South West

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
for the anisotropy ratios to be written to the 2nd BCF package (*.BC2) when a single anisotropy value is specified for each layer (ITRPY=0). Executable: 'mfwvk19' Modules: 'bcf5.f17' (based on 'bcf5.f16')	anisotropy ratios to the *.BC2 package when using a single anisotropy value for each layer (Allows anisotropy ratios to be specified for each layer (ITRPY=0) when using the automatic SpecT to VKD option (ISS=2)). Correction made so that the transmissivity output flag (ITRANS) is written to the *.BC2 package		Chilterns model.
22. Correction to the calculation of transmissivity when using nodal K values and VKD Executable: 'mfwvk20' Modules: 'bcf5.f18' (based on 'bcf5.f17')	The transmissivity calculation was corrected so that transmissivities are not overestimated when using the nodal transmissivity option (LAYAVG < 40).	No changes	Tested using South West Chilterns model.

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
23. Added progress monitor for PCG solver package & allow forced convergence. Executable: 'mfwvk21' Modules: 'pcg2.f02' 'Modflw96.f08' (based on 'pcg2.f01' (based on 'pcg2.for') and 'Modflw96.f07')	Added progress monitor that had been developed for another project (reproduced with permission from the Client). Allows the head change and flow residual to be monitored during a simulation when using the PCG solver. Also allows convergence to be forced if the convergence criteria are met for a specified number of outer iterations (NOUTC) (rather than having to converge in the first inner iteration).	Insert the number of outer iterations which must satisfy the convergence criteria before convergence is forced (NOUTC) between the 31st and 40th columns of the first row of the PCG file (same as GV).	Tested against mfwin32 using models from other project.
24. Allow no forced convergence if NOUTC is 0. Executable: 'mfwvk22' Modules: 'pcg2.f03' (based on 'pcg2.f02')	Only allows convergence to be forced if NOUTC is greater than zero.	Will now work with files that don't have a value for NOUTC (ie. Modflow96 files).	Tested using 'VKD6e-tv3'.

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
25. Use Tx and Ty directly. Executable: 'mfwvk23' Modules: 'bcf5.f19' 'modflw96.f09' (based on 'bcf5.f18' and 'modflw96.f08')	Changed the code so that if anisotropy flag (ITRPY) is set to 2, the code uses the X- and Y- direction transmissivities (or hydraulic conductivities) directly rather than calculating the anisotropy ratios, which can lead to errors when a zero transmissivity is specified in a cell. Had to change some code in SBCF5N to check conductances more thoroughly before making a node inactive.	No change (but can now enter zeros for transmissivity or hydraulic conductivity without errors).	Tested using 'swc008tv-test', 'SpecT1-test', 'SpecT2a-test', 'SpecT2b-test', 'SpecT1u-test', 'VKD3-test', 'VKD4-test', 'SpecT2u2-test', 'VKD4a-test', 'VKD4b-test', 'VKD4c-test', 'VKD5b-test' & 'VKD6c-test'. Main test: 'VKD5b-test2'
26. Use VMID (middle elevation). Executable: 'mfwvk24' Modules: 'bcf5.f20' 'modflw96.f10' (based on 'bcf5.f19' and 'modflw96.f09')	Changed the code to use a new array (VMID) rather than the old TOP array to specify the elevation at which hydraulic conductivity changes from constant to varying with depth. Also made some corrections so that ITRANS is written to the second BCF (BC2) file, and so that correct values are written for HDRY, TMP (head value for no-flow cells), WETFCT, PERLEN & TSMULT (previously values after the decimal point were lost).	Secondary storage coefficient (SC2) and TOP elevations are no longer read in when LAYCON is 4 (unconfined VKD). Instead VMID and VKGRAD are read in following all other arrays for the layer (i.e. after WETDRY if used – previously VKGRAD was read in between TOP and WETDRY).	'VKD5b-test3' & 'VKD4a-test2'.
27. Allow VKD in any layer (confined VKD: LAYCON = 5). Executable: 'mfwvk25' Modules: 'bcf5.f21' (based on 'bcf5.f20')	Introduced a new layer type to represent a VKD layer that can become confined (LAYCON = 5). Major changes to subroutine BCF5VK (code that produces new NA2, BA2 & BC2 files). Now performs an automatic conversion from a specified transmissivity run for layer types 1, 3, 4 & 5 (when ISS=2) *[this was later changed – see below]*. Reorganised inputs for this option so that bottom elevations are read rather than bottom zone thicknesses so that overlapping layers are not produced.	Inputs for a layer with a LAYCON value of 5 are identical to those for LAYCON = 4, but with a top elevation and a secondary storage coefficient. When using the automatic conversion option (ISS = 2) bottom elevations should be specified rather than thicknesses.	'VKD4a-test3', 'VKD5b-test4', 'VKD8', 'VKD9', 'VKD10', 'VKD11', 'VKD12', 'VKD13'

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
28. Include VKMAX Executable: 'mfwvk26' Modules: 'bcf5.f22' 'modflw96.f11' (based on 'bcf5.f21' and 'modflw96.f10')	Changed the code to use a new array (VKMAX) to specify a maximum hydraulic conductivity (in terms of the base hydraulic conductivity, i.e., if the base hydraulic conductivity (HY) is 8, and VKMAX is 3, then the maximum hydraulic conductivity is 24 (3 x 8)). More changes to subroutine BCF5VK (code that produces new NA2, BA2 & BC2 files). No longer performs an automatic conversion from a specified transmissivity run for layer types 1 and 3 (when ISS=2), only for layer types 4 and 5. Changed title for VKGRAD from "HYDRAULIC COND GRADIENT" to "HYD COND GRADIENT FACTOR".	Add the VKMAX array after the VKGRAD array.	'VKD14'
29. Adjust top thicks Executable: 'mfwvk27' Modules: 'bcf5.f23' (based on 'bcf5.f22')	Changed the code to automatically adjust top thicknesses if the values specified by the user are too high. A list of the values changed and the adjusted arrays of top thickness are printed to the (first) output file. Arrays of bottom thickness are also printed to the (first) output file.	None	'VKD15', 'VKD16', 'VKD-test003'
30. allow dry cells in first part of a SpecT->VKD simulation Executable: 'mfwvk28' Modules: 'bcf5.f24' (based on 'bcf5.f23')	Changed the code so that the layer type is no longer changed to 0 (confined), but that the transmissivity calculation is different if the automatic conversion option is activated (ISS=2). This means that the cells can become dry (and rewet) and that all the leakance corrections are also applied to the first part of the simulation, so that there should be differences between the first and second parts of the simulation. The subroutine SBCF5V is no longer used.	None	'VKD-test004'

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
31. changed to set property values to zero at dry cells Executable: 'mfwvk29' Modules: 'bcf5.f25' (based on 'bcf5.f24')	Changed the code so that cells that are dry are given property values of zero for the second part of the simulation (applies to HY, CV, TOP, WETDRY, VMID, VKGRAD, & VKMAX arrays at present). This means that if they become wet due to rewetting, they are immediately made inactive again (rather than allowing them to become active with incorrect property values). Note: should also give zero values to TRPY arrays, and to leakance arrays for layer above…	None	'VKD-test005'
32. changed to write CV values to output file Executable: 'mfwvk30' Modules: 'bcf5.f26' and 'modflw96.f12' (based on 'bcf5.f25' and 'modflw96.f11')	Changed code so that CV values are written to the output file along with internodal transmissivities if ITRANS=1. Also changed code so that the screen output unit is not closed between simulations. No longer get an error after the first simulation.	None	'VKD-test005'

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
33. changed to allow variable storage with depth (VSD) Executable: 'mfwvk31' Modules: 'bcf5.f27' and 'modflw96.f13' (based on 'bcf5.f26' and 'modflw96.f12')	Changed code to read in storage gradient factor array (VSGRAD) and maximum storage factor array (VSMAX). Changed code that calculates storage flows for the volumetric budget. Changed part of code that calculates contributions to the right hand side of the GW equation (RHS array) and the head dependant part (HCOF array). Due to nonlinear head dependence, the entire change in storage is added to the RHS, plus a term including the storage coefficient for the current GW head. The term for the current GW head is also added to the HCOF array. These two terms cancel each other out if the head remains the same and provides a close approximation if it doesn't. The terms are updated every (outer) iteration. Due to the approximation described above, the code had to be compiled using the additional flag, /DREAL, which changes all 'real' variables to 'double precision' variables. This is so that the terms including the storage coefficient for the current GW head in both the RHS and HCOF arrays balance exactly. Previously the HNEW array was 'double precision' but the RHS was only 'real'.	VSGRAD and VSMAX arrays added to BCF file after VKMAX array, if ISS (steady state flag) is zero.	'VKD7-tv3-test2', 'VKD7-tv3-test3', 'VKD7-tv3-test4', 'VKD7-tv3-test5'
34. changed to allow PCG debugger Executable: 'mfwvk32' Modules: 'pcg2.f04' and 'modflw96.f14' (based on 'pcg2.f03' and 'modflw96.f13')	Code changed to allow a debugging option, which produces a file of all the heads calculated in the iteration process. This file is reset each time that a time step converges, so that only the information from an unconverged time step is kept. The outer iteration number is written to the part of the file that usually contains the stress period number, the inner iteration no. to the time step location, the largest head change to the stress period time location, and the largest flow residual to the total time location.	The output file needs to be specified in the name file as DATA(BINARY), and the unit number should be entered in columns 41-50 in the 1st line of the PCG input file.	'VKD-test008tv'

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
35. changed to include VSMID array Executable: 'mfwvk33' Modules: 'bcf5.f28' and 'modflw96.f15' (based on 'bcf5.f27' and 'modflw96.f14')	Changed code to include a new array (VSMID) specifying the elevation of the change in storage ('point of inflection' for storage). This array is located after the VKMAX array and before the VSGRAD array. Storage calculations changed to use the VSMID array rather than the VMID array (elevation of change in hydraulic conductivity).	The VSMID array is added to the BCF file after the VKMAX array and before the VSGRAD array, if ISS (steady state flag) is zero.	'vkd7-tv3-test9'
36. changed format of HY & VMID arrays (auto-conv) Executable: 'mfwvk34' Modules: 'bcf5.f29' (based on 'bcf5.f28')	Changed code so that when the auto-conversion option is used, the hydraulic conductivity (HY), and elevation of change in hydraulic conductivity (VMID) arrays are written to the second BCF package (*.BC2) using the format: '(10E23.16)', whatever the format of the input arrays for transmissivity (HY) and upper thickness (VMID).	Means that the transmissivity and upper thickness arrays can be written to the first BCF file using any convenient format, and the results of the first and second simulations should be very nearly identical.	'ltch34'
37. changed to replace VKGRAD values of zero with VKMAX values of 1 Executable: 'mfwvk35' Modules: 'bcf5.f30' (based on 'bcf5.f29')	Changed the code so that it checks for hydraulic conductivity gradient factor (VKGRAD) values of zero (which would represent no variation of K with depth), and replaces them with values of 1.0 (Thus avoiding divide by zero errors). The corresponding maximum hydraulic conductivity factor (VKMAX) is also set to 1.0 so that there is no variation of K with depth. The locations of the changed values are written to the output file. Removed option in routine B12DRI to read integer arrays (this routine was causing errors during compilation – even though no changes had been made to that part of the code)	Means that zeros can be entered in the hydraulic conductivity gradient factor (VKGRAD) array, without producing errors.	'ltch35', 'ltch36'

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
38. improved writing of 2nd BCF file Executable: 'mfwvk36' Modules: 'bcf5.f31' (based on 'bcf5.f30')	Changed code that writes arrays to the second BCF file (when using the automatic conversion option: ISS=2) so that all arrays are checked for constant values (including 1-D arrays such as the column & row spacing) and all property values are set to zero for dry/no-flow cells. Changed code that writes inter-nodal transmissivities & leakances to the output file (if ITRANS is not 0) so that leakances are written for the lowest layer. Changed title for VMID array in second BCF file from 'MIDDLE ELEVATION' to 'ELEVATION OF CHANGE IN K'. Removed options to write storage property values to the second BCF file as these would never be written. Changed title for BOT array in first BCF file from 'LOWER THICKNESS' to 'BOTTOM' (no longer use lower thickness).	No changes to input required from the user	'ltch37'
39. allow auto-conversion of const-K layers Executable: 'mfwvk37' Modules: 'bcf5.f32' & 'modflw96.f16' (based on 'bcf5.f31' & 'modlfw96.f15')	Added a new option to convert constant K layers (LAYCON = 1 or 3) to VKD layers (LAYCON = 4 or 5) by setting the steady state flag (ISS) to 3. Changed code that assigns property names to different arrays, code that calculates transmissivity, and the code that calculates the base hydraulic conductivities. Also changed code in main program to call auto-conversion module if ISS = 3.	Can set steady state flag (ISS – first number in BCF file) to 3. This will mean that any layers specified as 4 or 5 will run as specified hydraulic conductivity before conversion to VKD. (old option of ISS = 2 runs these layers as specified transmissivity)	'ltch38', 'ltch37'

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
40. allow specified filenames for 2nd simulation Executable: 'mfwvk38' Modules: 'bcf5.f33' (based on 'bcf5.f32')	Added code to check for a ">" symbol following the filenames in the NAME file (LST, BAS, BCF, DATA and DATA(BINARY) file types only). If detected, a new filename is read which will be used for the second simulation. If the symbol is not present then the old convention of replacing the last letter of the filename with "2" is used (LST, BAS, BCF, and DATA(BINARY) file types only).	Can add specific filenames to the NAME file, which will be used in the second simulation.	'ltch38'
41. allow different formats for each layer array Executable: 'mfwvk39' modules: 'bcf5.f34' (based on 'bcf5.f33')	Increased the size of the FMTIN array so that a format is stored for each property array for each layer. This means that different formats can be used for each layer, and they will be reproduced in the 2nd BCF file. Also changed the code so that the format for the anisotropy ratio array is fixed at '(10E23.16)' if LAYCON is 4 or 5, and ITRPY is 2 or LAYAVG is 40. Removed some remaining references to storage in the auto-conversion routine. Added a line that skips the VKD parameter calculations if the cell is not active.	Means that arrays can be written to the first BCF file using any convenient format, and the results of the first and second simulations should be very nearly identical.	'ltch39'
42. allow single precision (REAL) variables Executable: 'mfwvk40' modules: 'bcf5.f35' (based on 'bcf5.f34')	Made some variables in subroutines 'BCF5FM' & 'SBCF5S' double precision (those relating to the storage calculations). Compiled the code without using the DREAL option (which changes all REAL variable types to DOUBLE PRECISION types). This change means that the binary file outputs will be around half the size that they were when the code was compiled using the DREAL option.	none	'vkd7-tv3-test10'

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
43. allow direct access binary files Executable: 'mfwvk41' modules: 'bcf5.f36' & 'utl5.f02' (based on 'bcf5.f35' & 'utl5.for')	Changed utilities that write the standard output to head, drawdown and cell-by-cell flow files, so that the file access for these is checked first, and the records written accordingly (note that the changes made to 'utl5.f01' (print formats) have not been incorporated into 'utl5.f02'). Change to code that writes the 2nd NAMe file to allow the DIRECT access option (the BAS & BCF files cannot be specified as direct access). This change allows output files to be created which can be read by GV without the need to convert the files after the simulation has run.	To create direct access binary output files (head, cbc, etc,.) that can be read by GV insert the keyword 'DIRECT' after the file name followed by the record length (a record length of 4 should work for all simulations – unless the code has been compiled using the DREAL option)	'vkd7-tv3-test10', 'ltch39'
44. clear old direct access binary files when overwriting Executable: 'mfwvk42' Modules: 'utl5.f03' (based on 'utl5.f02')	Change the code to check when the first record of a standard direct access binary output file (i.e. *.hds, *.ddn, *.cbc, etc.) is being written. When it is, the file is closed and deleted and re-opened using the original filename and record length. This change avoids overwriting part of an old binary file with new data – with the possibility of the old data being mistaken for the new.	none	'ltch41', 'ltch41tv'
45. changed to replace VSGRAD values of zero with VSMAX values of 1 Executable: 'mfwvk43' Modules: 'bcf5.f37' (based on 'bcf5.f36')	Changed the code so that it checks for storage gradient factor (VSGRAD) values of zero (which would represent no variation of S with depth), and replaces them with values of 1.0 (Thus avoiding divide by zero errors). The corresponding maximum storage factor (VSMAX) is also set to 1.0 so that there is no variation of S with depth. The locations of the changed values are written to the output file.	Means that zeros can be entered in the storage gradient factor (VSGRAD) array, without producing errors.	'ltch41tv'

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
46. automatically calculate record length of direct access binary files Executable: 'mfwvk44' Modules: 'utl5.f04' (based on 'utl5.f03')	Changed the code to re-open direct access binary files (before writing the first record) with the correct record length. This means that the correct record length does not need to be calculated by the user and specified in the NAMe file, although a number should be entered after the keyword 'direct' (a value of 1 should avoid any possible errors). This is also quicker than entering a record length of 4, which increased run times by around 50%.	To create direct access binary output files (head, cbc, etc,.) that can be read by GV insert the keyword 'DIRECT' after the file name followed by an integer (a value of 1 should work for all simulations)	'ltch41tv'
47. allow stream inflows, outflows and tributaries at any reach Executable: 'mfwvk45' Modules: 'str1.f03' and 'modflw96.f17' (based on 'str1.f01' and 'modflw96.f16')	Changed the stream package to allow new options. New flag (ISWABS) on first line of stream input file (columns 81-90): ISWABS = 0. Original Modflow96 formulation (not including modification to 'str1.f01'). Inflows only allowed for first reach in a segment, tributary inflows identified by negative inflow value. ISWABS < 0. Specified discharges and abstractions are allowed in any stream reach. Abstractions are limited by the flow available in the stream (will take all flow available if flow is less than the abstraction rate), messages are written to the output file if the abstraction is reduced. Tributary inflows are specified by the tributary definitions section, and are always routed to the first reach of a stream segment (no need to identify with negative inflow value). ISWABS > 0. Same as for ISWABS < 0 except tributary inflows can be specified for any reach of a stream segment. Extra numbers are required in the tributary definitions section. Before each number specifying which segment flows into each segment, the reach number of the destination segment is specified. Each reach and segment number occupies 5 columns of the input file.	Enter a value for ISWABS in columns 81 to 90 of the first line of the stream input file. If ISWABS is zero or blank, the original input format is used. If ISWABS is not zero, positive or negative flows can be specified for each stream reach. Negative numbers are not required for locations of tributary inflows. If ISWABS is positive, the reach number at which tributaries enter a stream segment must be specified before the segment number of the tributary (both numbers are integers of 5 characters length).	'ltch42tv' to 'ltch47tv'

Purpose of changes & filenames for new code	Description of code changes & Rational	Changes to MODFLOW input files	Testing procedures
48. Corrections to auto-conversion routine Executable: 'mfwvk46' Modules: 'bcf5.f38' (based on 'bcf5.f37')	Changed the code in the auto-conversion routine to set the format for the initial heads array to '(10E23.16)' rather than using the input format. This will make the second simulation more likely to converge. Also changed the code so that the correct title is written to the output file for the lower thicknesses.	None (although a high degree of precision is not now needed for the initial heads array in the BASic input file for an auto-conversion simulation).	'ltch47'
49. Increased size of X-array Executable: 'mfwvk47' Modules: 'modflw96.f18' (based on 'modflw69.f17')	Increased the size of the X-array from 2,000,000 to 10,000,000 following a request from Simon Quinn at Entec.	None	
50. modified binary output of accreted stream flows Executable: 'mfwvk48' Modules: 'str1.f04' (based on 'str1.f03')	The output of accreted stream flows to the binary cell-by-cell flow file was modified so that, if there is more than one stream reach in the same cell, only the accreted flow from the reach furthest downstream (furthest down the list in the input file) is saved.	None (Binary output of accreted flows will change if more than one stream reach is specified in any one cell).	'str-dewat-inj' (test model)

There were only a few small changes that were made since mfwvk47.exe:

1. A minor one to the stream package so that if more than one stream reach is specified in a model cell, and accreted stream flows are being written to a binary cell-by-cell flow file, only the accreted flow from the furthest downstream reach is recorded (previously the sum of the accreted flows of all the reaches in that cell was reported).
2. A change in the handling of the PCG debug output file so that the file is cleared each time a timestep converges (see the user guide for a description of the PCG debug file).
3. A change to the way that direct access binary files are cleared when the first record is written to them, to avoid possible errors with opening and closing files with certain combinations of fortran compiler and operating system.
4. Removed an obsolete subroutine from the BCF package (one that was previously used in the auto-conversion routine).
5. Changed code that reads name the file so that filenames for the second simulation (if using auto conversion option - see User Guide) are not changed to upper case.
6. Updated the titles printed for each package at the start of the listing output file.
7. Improved comment lines in source code.

APPENDIX B
Modelling log

MODELLING LOG

Project Number: 1621
Project Name: Enhancements to Modflow 1
Modeller: Adam Taylor
Start Date: 02/10/2000

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'VKD5e' 24/10/00 Based on 'VKD5' Reduced thickness of upper zone to zero. Version of MODFLOW used: Mfwvk21.exe	Reduced thickness of upper zone to zero (so that the GW heads will fluctuate around the elevation at which the hydraulic conductivity changes from constant to varying in the subsequent time variant simulation – to check the stability when heads are at this elevation)	'Top' elevations = steady state heads at each node	Used as initial heads for 'VKD6e-tv3'
'VKD6e-tv3' 24/10/00 Based on 'VKD6-tv3' Reduced thickness of upper zone to zero. Versions of MODFLOW used: Mfwvk21.exe Mfwvk22.exe	Reduced thickness of upper zone to zero (so that the GW heads will fluctuate around the elevation at which the hydraulic conductivity changes from constant to varying – to check the stability when heads are at this elevation) Used Top, Bottom and hydraulic conductivity arrays from 'VKD5e.bc2' (created during last simulation). Set IHOLD and ITRANS to 1 NOUTC (in PCG package) set to zero.	Total number of iterations increased from 1225 ('VKD6-tv3') to 1242. Very little change to flow balance errors Calculation of transmissivity checked for cell (5,5) in timestep 1 of stress period 30- OK ('Check-T.xls').	Simulation takes a little longer to converge when heads are at the elevation of the change from constant to varying hydraulic conductivity.
'swc008tv-test' 25/10/00 Based on 'swc008tv' No changes Version of MODFLOW used: Mfwvk23.exe	No changes – used to test new version of code.	Produces identical results to 'swc008tv'	

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'SpecT1-test' 25/10/00 Based on 'SpecT1' No changes Version of MODFLOW used: Mfwvk23.exe	No changes – used to test new version of code.	Maximum head difference compared to 'SpecT1' is 4.6e-5 m.	
'SpecT2a-test' 25/10/00 Based on 'SpecT2a' No changes Version of MODFLOW used: Mfwvk23.exe	No changes – used to test new version of code.	Produces identical results to 'SpecT2a'.	
'SpecT2b-test' 25/10/00 Based on 'SpecT2b' No changes Version of MODFLOW used: Mfwvk23.exe	No changes – used to test new version of code.	Produces identical results to 'SpecT2b'.	
'SpecT2u-test' 25/10/00 Based on 'SpecT2u' No changes Version of MODFLOW used: Mfwvk23.exe	No changes – used to test new version of code.	Maximum head difference compared to 'SpecT2u' is 7.6e-6 m.	

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'SpecT1u-test' 25/10/00 Based on 'SpecT1u' No changes Version of MODFLOW used: Mfwvk23.exe	No changes – used to test new version of code.	Maximum head difference compared to 'SpecT1u' is 7.6e-6 m.	
'VKD3-test' 25/10/00 Based on 'VKD3' No changes Version of MODFLOW used: Mfwvk23.exe	Used to test new version of code. Changed input formats to '(_e14.5)' to match the automatic formats given to the *.BA2 & *.BC2 files created by the older version of the code. Set ITRANS to 1 to output transmissivities to output file.	Maximum head difference compared to 'VKD3' is zero for the first part of the simulation, and 1.5e-3 m for the second.	Relatively large differences in the results of the second part of the simulation are probably due to the fact that 'VKD3' was run using versions of MODFLOW ('mfwvk4' & 'mfwvk5') that automatically used the initial heads to calculate the transmissivity for steady-state VKD simulations. This has since been corrected.
'VKD4-test' 26/10/00 Based on 'VKD4' No changes Version of MODFLOW used: Mfwvk23.exe	No changes – used to test new version of code.	Maximum head difference compared to 'VKD4' is zero for the first part of the simulation, and 1.1e-2 m for the second.	See comment above. Also input formats not updated as they were in the previous run. Re-run with modified 'mfwvk23.exe' – results unchanged.
'SpecT2u2-test' 26/10/00 Based on 'SpecT2u2' No changes Version of MODFLOW used: Mfwvk23.exe	No changes – used to test new version of code.	Produces identical results to 'SpecT2u2'.	

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'VKD4a-test' 26/10/00 Based on 'VKD4a' No changes Version of MODFLOW used: Mfwvk23.exe	No changes – used to test new version of code.	Maximum head difference compared to 'VKD4a' is zero for the first part of the simulation, and 1.2e-2 m for the second.	See comments above. Re-run with modified 'mfwvk23.exe' – results unchanged.
'VKD4b-test' 26/10/00 Based on 'VKD4b' No changes Version of MODFLOW used: Mfwvk23.exe	No changes – used to test new version of code.	Maximum head difference compared to 'VKD4b' is zero for the first part of the simulation, and 1.8e-2 m for the second.	See comments above. Re-run with modified 'mfwvk23.exe' – results unchanged.
'VKD4c-test' 26/10/00 Based on 'VKD4c' No changes Version of MODFLOW used: Mfwvk23.exe	No changes – used to test new version of code.	Maximum head difference compared to 'VKD4c' is zero for the first part of the simulation, and 1.8e-2 m for the second. Identical to previous run as LAYAVG is automatically changed from 3X to 2X.	See comments above. Re-run with modified 'mfwvk23.exe' – results unchanged.
'VKD5b-test' 26/10/00 Based on 'VKD5b' No changes Version of MODFLOW used: Mfwvk23.exe	No changes – used to test new version of code.	Maximum head difference compared to 'VKD5b' is zero for the first part of the simulation, and 6.6e-3 m for the second. Code had to be corrected to make this run work (SBCF5V & SBCF5N). Therefore re-ran 'VKD4' and 'VKD4a' to 'VKD4c' (results OK).	See comments above. Re-run with modified 'mfwvk23.exe' – results unchanged.

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'VKD6c-test' 26/10/00 Based on 'VKD6c' No changes Version of MODFLOW used: Mfwvk23.exe	No changes – used to test new version of code.	Produces identical results to 'VKD6c'.	
'VKD5b-test2' 02/11/00 Based on 'VKD5b-test' Using zero transmissivities. Version of MODFLOW used: Mfwvk23.exe	Changed last column of X-direction transmissivities to zero (not used when LAYAVG=40) Changed last row of Y-direction transmissivities to zero (not used when LAYAVG=40)	Identical results to 'VKD5b-test' Code had to be corrected to make this run work (SBCF5N). Previously the code was making nodes inactive because it thought that all it's conductances were zero. Changes had to be made to the code & tested using this model (no previous models had any zero transmissivities or hydraulic conductivities).	
'VKD5b-test3' 06/11/00 Based on 'VKD5b-test2' No changes. Version of MODFLOW used: Mfwvk24.exe	No changes – used to test new version of code.	Maximum head difference compared to 'VKD5b' is zero for the first part of the simulation, and 6.6e-3 m for the second (transmissivity calculations in code have been changed slightly).	
'VKD4a-test2' 06/11/00 Based on 'VKD4a-test' No changes Version of MODFLOW used: Mfwvk24.exe	No changes – used to test new version of code.	Maximum head difference compared to 'VKD4a' is zero for the first part of the simulation, and 1.15e-2 m for the second.	

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'VKD4a-test3' 07/11/00 Based on 'VKD4a-test2' Changed bottom thicknesses to elevations Version of MODFLOW used: Mfwvk25.exe	Changed the bottom thickness array to bottom elevations (copied array from 'VKD4a-test2.bc2').	Maximum head difference compared to 'VKD4a' is zero for the first part of the simulation, and 1.1e-2 m for the second. Hydraulic conductivities written to the BC2 file are slightly higher to the right hand side of the model.	
'VKD5b-test4' 07/11/00 Based on 'VKD5b-test3' Replaced bottom thicknesses with elevations Version of MODFLOW used: Mfwvk25.exe	Replaced bottom thicknesses with elevations (from 'VKD5b-test3.bc2').	Maximum head difference compared to 'VKD5b' is zero for the first part of the simulation, and 4.8e-3 m for the second (hydraulic conductivity calculations in code have been changed slightly).	
'VKD8' 07/11/00 Based on 'VKD5b-test4' Set layer type to confined VKD Version of MODFLOW used: Mfwvk25.exe	Set layer type (LAYCON) to 5 Added TOP array at 200m throughout model (above all GW heads).	Identical results to 'VKD5b-test4'	
'VKD9' 07/11/00 Based on 'VKD8' Two layer model Version of MODFLOW used: Mfwvk25.exe	Two layer model: Upper layer is unconfined VKD (LAYCON=4) Lower layer is convertible VKD (LAYCON=5) Identical properties in each layer Top of lower layer set to 200m (above GW heads) Leakance (VCONT) between layers = 0 Output control changed so that only heads and drawdowns for layer 2 are saved to the binary files (makes comparisons with previous runs easier) (Layers are actually set at same elevation etc – not realistic system(!) but ok to test numerics of code)	Heads in layer 2 are identical to those from 'VKD5b' in the first part of the simulation, and are different by 4.8e-3 m in the second. Heads in layer 2 are identical to those in layer 1 to at least 7 decimal places.	Layer type 5 works fine when it is unconfined (still need to test it under confined conditions). Automatic conversion works fine for a two layer model with layer types of 4 and 5.

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'VKD10' 08/11/00 Based on 'VKD9' Upper layer confined Version of MODFLOW used: Mfwvk25.exe	Two layer model: Upper layer is confined (LAYCON=0) Bottom elevation, thickness of upper zone, & hydraulic conductivity gradient factor removed from properties of layer 1 (BCF package).	Heads in layer 2 are identical to those from 'VKD5b' in the first part of the simulation, and are different by 4.8e-3 m in the second.	Layer type 5 works fine when it is below a confined layer. This means that all the layer counters relating to top, bottom and middle elevations are working ok. Automatic conversion works fine for a two layer model with layer types of 0 and 5.
'VKD11' 08/11/00 Based on 'VKD9' Upper layer convertible Version of MODFLOW used: Mfwvk25.exe	Two layer model: Upper layer is convertible (LAYCON=3) Thickness of upper zone, & hydraulic conductivity gradient factor removed from, & top elevation added to properties of layer 1 (BCF package). hydraulic conductivity gradient factor set to 0 for layer 2 Output control changed to save heads and drawdowns for both layers.	Results of layers 1 & 2 are identical to at least 4 decimal places in the first part of the simulation, and to at least 6 dps in the second.	Automatic conversion works fine for a two layer model with layer types of 3 and 5 (auto conversion also calculates hydraulic conductivities for LAYCON = 3 type layers – this feature was subsequently removed).
'VKD12' 08/11/00 Based on 'VKD11' Changed top & bottom elevations Version of MODFLOW used: Mfwvk25.exe	Two layer model: Tops of both layers set to 100 m Bottoms of both layers set to 50 m	Results of layers 1 & 2 are identical to at least 4 decimal places in the first part of the simulation, and to at least 6 dps in the second.	Transmissivity calculations are ok for LAYCON = 5 when heads are above the top of the layer
'VKD13' 08/11/00 Based on 'VKD12' VKGRAD set to 0.6 Version of MODFLOW used: Mfwvk25.exe	Two layer model: VKGRAD of layer 2 set to 0.6 per meter.	Results identical to 'VKD12' in first part of simulation. Different by 6.9e-5 for second part of simulation in layer 1 Different by 1e-3 for second part of simulation in layer 2	Confirms comment above

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'VKD14' 20/11/00 Based on 'VKD9' VKMAX array added Versions of MODFLOW used: Mfwvk26.exe Mfwvk27.exe	Two layer model: Added VKMAX arrays for both layers. Values of VKMAX set arbitrarily high (100.0) so that they shouldn't affect the calculations. Run using new version of code.	Results identical to 'VKD9'	VKMAX array does not affect simulation results when set to an arbitrarily high value
'VKD15' 21/11/00 Based on 'VKD14' Top thickness=100 Versions of MODFLOW used: Mfwvk27.exe	Two layer model: Top thickness set to 100 (greater than total thickness) for both layers. To test the automatic adjustment of layer thicknesses.	Results identical to 'VKD14' in first part of simulation. Different by 6.1e-3 in second part.	Automatic adjustment of layer thicknesses works OK (still get some lower thicknesses in some areas of +/- 3.815e-06 – result of mixed single and double precision calculations? – wouldn't effect second part of simulation unless BOT or VMID arrays are written to 6 decimal places or more!)
'VKD16' 21/11/00 Based on 'VKD11' VKMAX added with value of 1.0 Versions of MODFLOW used: Mfwvk27.exe Mfwvk28.exe	Two layer model: Added the VKMAX array with a value of 1.0 (max K = base K).. Set VKGRAD to 0.6.	Results from layer two different from layer two of 'VKD11' by 7.6e-5 in the first part of the simulation, and by 2.3e-4 in the second (results of layer one are vastly different due to the removal of the automatic conversion option for layer type 3). Calculated hydraulic conductivities identical to 4 significant figures to those in 'VKD11' (except in one location – difference of 0.01).	VKMAX works in limiting the hydraulic conductivity to a maximum value.

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'VKD-test001' 23/10/00 New test model Versions of MODFLOW used: MFWin32	New test model: 50 rows, 30 columns, 1000m grid spacing. 3 layers dipping to south (slope=1/200), Top layer unconfined (LAYCON=1), middle layer convertible (LAYCON=3) with thickness of 30m, bottom layer convertible with thickness of 70m. Base of layer 1 to the north is at 210m AD. Kx = Ky = Kz = 30 m/d throughout all layers. Leakance between layers calculated from Kz & layer geometry (uses initial heads in layer 1). Initial heads set at 300m AD. River cells form main outflow along southern boundary of layer 1: conductance = 10,000 m^2/d, stage = 5m, bottom = 0m. Stream cells represent two streams flowing north to south, which meet at the centre, 8km north of the southern boundary: Both streams start in layer 3 to the north, and move into layers 2 and 1 towards the south. Western stream has around two or three times the gradient of the eastern stream (1 in 1000). Conductance = 10,000 m^2/d, bottom = stage. Recharge applied at a rate of 5e-4 m/d; except in area around centre of model where recharge is zero. There are also no stream cells in this area of the model, which represents an area of low permeability drift. Resaturation active: wetting factor=1, wetting threshold=0.1, head for dry cells=-888, wetting iteration interval=5, eqn no.=0, option=use only node below dry cell: PCG solver: max outer iterations=1000, max inner iterations=5, Hclose=0.001, Rclose=0.1, relax=1, precond method=Cholesky, max bound on eigenvalue=2, printing option=all, summary data every 5 timesteps, damp=1, force convergence if criteria met for 9999 outer iterations.	Model run using standard modflow (windows version: MFWin32). Active flow zone within model determined from drying and rewetting of cells. Most of layer 1 becomes dry, half of layer 2, and a small area to the north of layer 3.	Layer 1 does not go dry immediately north of the last stream cells in this layer. There are a couple of cells north of the last stream cells which are still active. These cells are above the stream cells in layer 2, which although initially counter intuitive, could be thought of as representing groundwater flow in the river banks above the stream, within a kilometre of the stream.
'VKD-test002' 21/11/00 based on 'VKD-test001' changed K distribution Version of MODFLOW used: MFWin32	Changed hydraulic conductivity (K) distribution: High K of 150 m/d at locations of river and stream cells (all layers), K reduces away from streams to minimum of 1 m/d at interfluves.	Similar distribution of dry cells, steeper head gradients at interfluves.	

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'VKD-test003' 21/11/00 based on 'VKD-test002' VKD version of model Version of MODFLOW used: Mfwvk27.exe	Changed layers types from 1,3 & 3 to 4,5 & 5. ISS (steady state flag) changed from 1 to 2 (automatic conversion option). Transmissivities set equal to hydraulic conductivities of last model multiplied by 20 in layers 1 & 2, and by 70 in layer 3. Hydraulic conductivity gradient factor (VKGRAD)=0.6 /m Maximum hydraulic conductivity factor (VKMAX)=5 Resaturation inactive.	No dry cells appear in the first part of the simulation because the layer types are changed to 0 for this part of the simulation. Therefore heads from the second part of the simulation are significantly different from those of the first.	Need to change the code to allow dry cells in the first part of the simulation.
'VKD-test004' 21/11/00 based on 'VKD-test003' Run using new version of code Version of MODFLOW used: Mfwvk28.exe	Transmissivity output flag (ITRAN) set to 1 Run using new version of code: mfwvk28.exe	Second simulation failed to converge	
'VKD-test005' 23/11/00 based on 'VKD-test004' New version of code & changes to BCF file Versions of MODFLOW used: Mfwvk29.exe Mfwvk30.exe	Rewetting active: wetting interval=3 iterations, wetting threshold =-5m (cell below only), all other options as for 'VKD-test001'. Precision of transmissivity & upper thickness values (& hence hydraulic conductivity & middle elevation values in second simulation) & initial heads increased from 10e12.4 to 10e24.16. Hydraulic conductivity gradient factor (VKGRAD) increased to 1.0 /m. Multiplying factor for transmissivity in each layer set to 10 (was 20,20 & 70).	Second simulation converges on the same solution as the first.	Code working well. Important to increase precision of transmissivity, upper thickness and initial head arrays.
'VKD7-tv3-test' 07/12/00 based on 'VKD7-tv3' Rearrange slightly and use new code Version of MODFLOW used: Mfwvk30.exe	Rerun of the Stage II model: VKD7-tv3 Removed Secondary Storage array (no longer used for LAYCON=4 – was set to the same value as the primary storage coefficient, so this should not make a difference to the results). Added maximum hydraulic conductivity factor (VKMAX) with value of 10 (too high for it to affect the transmissivity calculations).	Maximum difference in head compared to 'VKD7-tv3' was 9.85e-3 m at row 3, column 15, during time step 1 of stress period 44. (2019 iterations in total)	New code gives same results for time variant simulations as old code (mfwvk18.exe) and the BHAM code (against which VKD7-tv3 was compared).

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'VKD7-til' 07/12/00 based on 'VKD7-tv3-test' Time instant steady state run Version of MODFLOW used: Mfwvk30.exe	Took storage flows for first time step from 'VKD7-tv3-test.cbc' (using 'heads2gv2.exe' to create 'VKD7-tv3-test-cbc.dat') and added these flows (converted to m/d) to the recharge (copied from 'VKD7-tv3-test.rch' – see 'VKD7-TV3-TEST-Sy-equiv-Rch.xls'). Changed the number of stress periods and time steps to 1. Changed steady state flag to 0.	Maximum difference in heads = 0.42m (relatively large difference is not due to number of significant figures for storage flows, but may be to do with the way that the storage flows are calculated in modflow (i.e. using single precision heads))	Experiment in using time instant steady state (TISS) and storage equivalent recharge (SER) partially successful.
'VKD7-tv3-test2' 18/12/00 based on 'VKD7-tv3-test' Add storage gradient, and maximum factors, and use new code Version of MODFLOW used: Mfwvk31.exe	Added storage gradient factor array (VSGRAD) = 1.0 Added maximum storage factor (VSMAX) = 1.0 All other inputs the same as 'VKD7-tv3-test' Run using new code. As VSMAX=1.0 the results should be identical to those from 'VKD7-tv3-test'	Maximum difference in head compared to 'VKD7-tv3' was 4.58e-5 m at row during stress periods 37 to 39. (2019 iterations in total)	New code gives same results for time variant simulations as old code (mfwvk30.exe) and the BHAM code (against which VKD7-tv3 was compared) when VSMAX=1.0.
'VKD7-tv3-test3' 19/12/00 based on 'VKD7-tv3-test2' increased maximum storage factor from 1 to 2 Version of MODFLOW used: Mfwvk31.exe	Increased maximum storage factor (VSMAX) from 1.0 to 2.0 All other inputs the same as 'VKD7-tv3-test'	Compared time variant flows with those from 'VKD7-tv3-test2': Less contribution to or from storage at beginning of dry or wet periods, more contribution towards middle and end of wet & dry periods. Less variation in river flows: due to less variation in groundwater heads. (1883 iterations in total)	Results make sense, but need a more rigorous method of testing the implementation of VSD…
'VKD7-tv3-test4' 19/12/00 based on 'VKD7-tv3-test3' increased maximum storage factor from 2 to 20 Version of MODFLOW used: Mfwvk31.exe	Increased maximum storage factor (VSMAX) from 2.0 to 20.0 All other inputs the same as 'VKD7-tv3-test'	Compared time variant flows with those from 'VKD7-tv3-test3': Results as above but more pronounced. (5868 iterations in total) Also tested water balance against spreadsheet calculations (based on the heads and properties at each node) see "VKD7-tv3-test4-Storage.xls". This gave the same results as reported in the MODFLOW output.	Results checked against spreadsheet. VSD works in single-layer unconfined model.

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'VKD7-tv3-test5' 21/12/00 based on 'VKD7-tv3-test4' Confined VKD with S=Sy Version of MODFLOW used: Mfwvk31.exe	Changed layer type to confined VKD (LAYCON=5). Added top array = initial heads array Added secondary storage array = primary storage array (1%)	Compared time variant flows with those from 'VKD7-tv3-test4': Smaller flows from storage & more variation in heads towards end of recharge periods. (5868 iterations in total) When the same simulation was tried with smaller confined storage coefficients the model failed to converge. Therefore, probably can't have very large changes in storage (this model changes from ~10% to 1%)	Looks like VSD works in single-layer confined model. Although this hasn't been checked so thoroughly (i.e. with spreadsheet as above).
'VKD-test005tv' 16/01/01 based on 'VKD-test005' time variant run Version of MODFLOW used: Mfwvk31.exe	Added recharge sequence: (1 constant year, 3 variable years) Extended river and stream files (constant props) 48 stress periods, 1 month each, 14 time steps each with multiplier of 1.5. VSMAX=1.0 No pumping Specific yield = 0.3% (0.003) Confined storage coeff = 0.0001	Converged OK	
'VKD-test006tv' 16/01/01 based on 'VKD-test005tv' with VSD Version of MODFLOW used: Mfwvk31.exe	Lots of combinations of parameters tried (storages, solver, and time step parameters)	Even with very low values for storage gradient factor (VSGRAD) and confined storage values close to specific yield values, the simulation failed to converge - often in the constant recharge part of the simulation (when heads shouldn't change!). Main problem appears to be in layer 3 (largest head change and residuals), so it seems unlikely that the problem is to do with large hydraulic conductivity values (only in layers 1 & 2). Also, no cells have changed from dry to wet or vice versa, so rewetting isn't the problem either…	VSD makes simulations very unstable

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'VKD7-tv3-test6' 16/01/01 based on 'VKD7-tv3-test5' VKMAX=VSMAX=1 Version of MODFLOW used: Mfwvk31.exe	Changed maximum hydraulic conductivity factor (VKMAX) to 1 Changed maximum storage factor (VSMAX) to 1 Effectively the same as Laycon=3	For comparison with next simulation	
'VKD7-tv3-test7' 16/01/01 based on 'VKD7-tv3-test6' Laycon=3 Version of MODFLOW used: Mfwvk31.exe	Changed layer type (LAYCON) to 3 Removed VKD & VSD parameters	Results identical to previous run	Changes to code have not affected the way storage changes from confined to unconfined.
'VKD7-tv3-test8' 16/01/01 based on 'VKD7-tv3-test5' top=1000 Version of MODFLOW used: Mfwvk31.exe	Set top to 1000 (above groundwater heads). Should give same results as 'VKD7-tv3-test4'	Results identical to 'VKD7-tv3-test4'	Layer type 5 behaves in exactly the same way as layer type 4 when heads are below the top of the layer.
'VKD-test007tv' 16/01/01 based on 'VKD-test006tv' using SIP solver Version of MODFLOW used: Mfwvk31.exe	Used SIP solver to see if this would converge better. Sy = 1% S gradient factor =0.1 'Confined' storage coefficient 1.5% (upper thickness = 5 m)	Crashed in first time step of variable recharge year.	SIP solver provides no advantage over the PCG solver with the 3-layer test model

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'VKD-test008' 16/01/01 based on 'VKD-test005' VKMAX = 1.0 (const K) Version of MODFLOW used: Mfwvk31.exe	Set VKMAX to 1.0 to see if the model would converge with constant K with depth.	Converged – used as initial conditions for 'VKD-test008tv'	
'VKD-test008tv' 17/01/01 based on 'VKD-test008' & 'VKD-test007tv' time-variant const-K run Version of MODFLOW used: Mfwvk31.exe	Set VKMAX to 1 (constant k)		Model discontinued as it was considered to be too complex to test the code – continuing with variations on the old stage II model.
'VKD7-tv3-test10' 22/02/01 based on 'VKD7-tv3-test2' added VSMID array Version of Modflow used: Mfwvk40.exe Mfwvk41.exe	Copied VMID array to VSMID array in BCF package Changed title text in BAS package Run using new version of code (that isn't compiled using the DREAL option) Should give same results as 'VKD7-tv3-test2' (for run using 'mfwvk41.exe': Changed name file so that head and drawdown filenames are followed with the keywords: 'DIRECT 4'. This means that the head & drawdown files are written in GV compatible format).	Once heads were converted to GV format and compared with those from 'VKD7-tv3-test2-GV.hds', the maximum difference was found to be 6.1e-5 m.	Single precision (REAL) version of code works fine – don't need to compile the code using the DREAL option (this will effectively half the size of the binary output files).

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'VKD7-tv3-test11' 22/05/01 – 29/05/01 based on 'VKD7-tv3-test5' added VSMID array, top=135, S=Sy/100 Version of Modflow used: Mfwvk48.exe	Copied VMID array to VSMID array in BCF package Set confined S = Sy/100 Set top elevation to 115m Changed title text in BAS package Run using new version of code Used various combinations of solver parameters and time step setup. Wouldn't work so tried following investigation: Set top to 190, relaxed convergence criteria (by factor of 100), set max outer iterations to 1000, set S=Sy, VSGRAD=0, VSMAX=1 (VSD not active). • Tried reducing inner iterations from 5 to 1 – total number of iterations increased from 1624 to 1957. • Reduced DAMP from 0.99 to 0.98 – its up to 1985 • Increased DAMP from 0.99 to 1 – its down to 1925 • Reduced top elev to 130m – its up to 1927 • Reduced top elev to 125m – its down to 1926 • Reduced top elevation to 120m – failed in SP 36 • Inner iterations increased from 1 to 5 – failed in SP 36 • Reduced VKGRAD from 0.6 to 0.4 – failed in SP 37 • Reduced VKGRAD from 0.4 to 0.3 – its down to 1592 • Increased VSGRAD to 0.1 & VSMAX to 1.5 – failed in SP 34 (VSD active) • Reduced VKGRAD to 0 – its up to 2802 (VKD not active) • Reduced elevation of change in S by 1 m – its down to 1502 • S=Sy/10 – failed in SP15 • Top=130 – failed in SP35 • VSMAX=1.6 – failed in SP1 • VSMAX=1.4 – failed in SP37 • Top=140 – its down to 1472 • Top=135 – its up to 1631 • S=Sy/100 – its up to 1753 • VKGRAD=0.1,VKMAX=1.1 – its down to 1710 (VSD and VKD active) • VKMAX=1.3 – its down to 1697 (VSD and VKD active)		Still having real problems with VSD. These problems become easier if you ensure that the elevations of the change in K and change in S are different, and if the layer is confined the S and K should meet their maximum values before the top of the layer.

Purpose of changes & filename	Description of changes and Rational	Effects of changes	Comments
'VKD7-tv3-test12' 09/07/01 based on 'VKD7-tv3-test' Added VSD Version of MODFLOW used: 'mfwvk48.exe'	Added change in Storage 10m below steady state head level Halved base Storage value vSgrad = 0.1/m, vsmax =3 Storage should be at original values at steady state head level. PCG package: Relaxed convergence criteria to 10^{-5} m for head changes and 10^{-2} m^3/d for flow residual. Maximum outer iterations set to 5000 Maximum inner iterations set to 1 Relaxation parameter set to 0.95	Failed to converge in time step 1 of stress period 35 (best that could be achieved!) Peaks and troughs in head lowered slightly compared to 'VKD7-tv3-test', intermediate levels increased slightly. Similar trend for flows to river.	

APPENDIX C
Results of pumping test models and discrete Cooper-Jacob analysis

Appendix C
Results of Pumping Test Models and Discrete Cooper-Jacob Analysis

Simple pumping test models were constructed to compare the responses of different types of aquifer (constant T, constant k, VKD, and VKD/VSD) to a pumping test. A way of analysing pumping test results to determine changes in hydraulic conductivity with depth was suggested from the modelling.

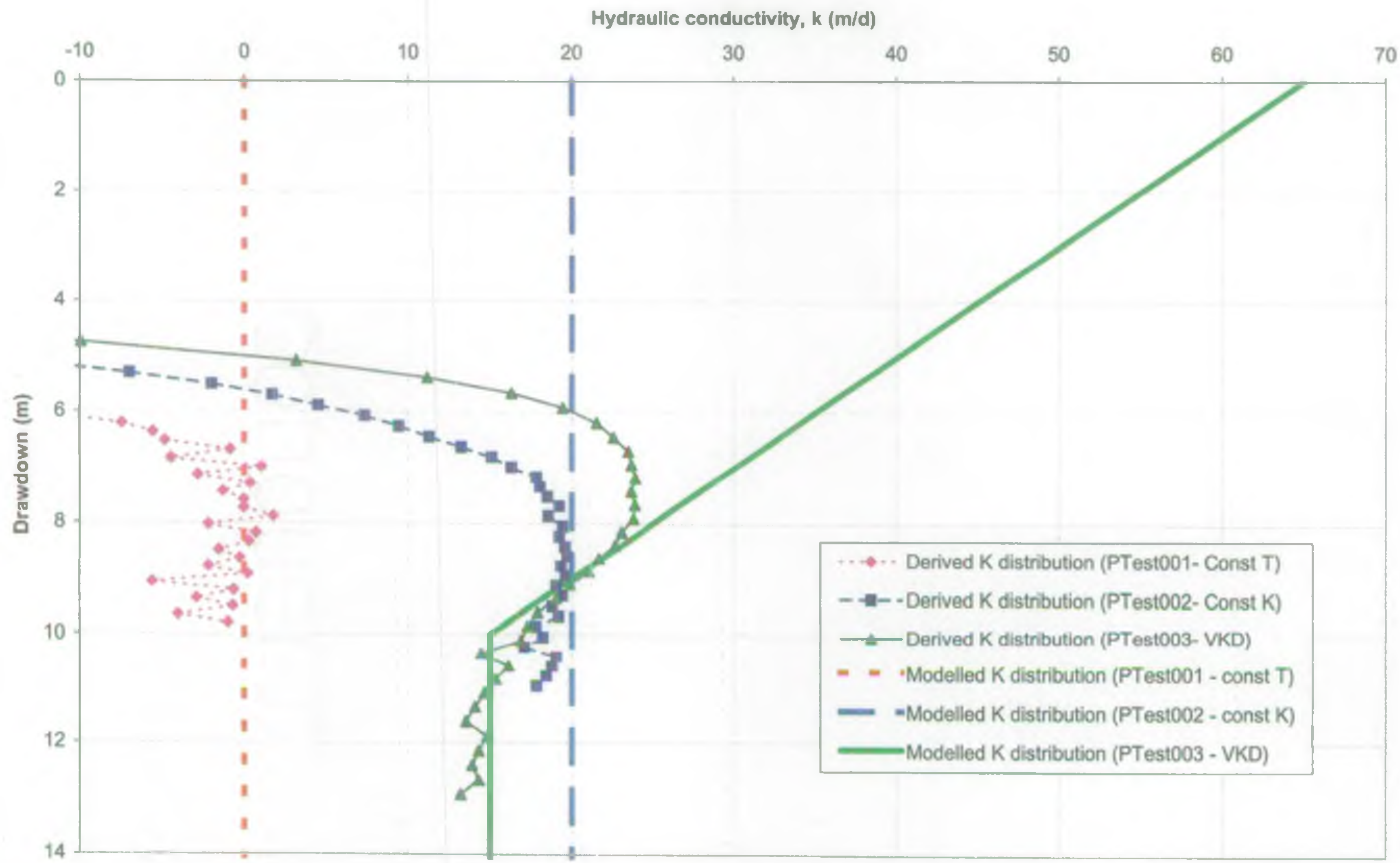
The models were based on a single layer grid of around 20 km by 20 km, with grid dimensions reducing from 3.3 km at the edge of the model to 0.1 m at the central cell representing the pumping borehole. The simulations were set up to pump at 10,000 m^3/d for 20 days followed by 20 days of recovery. The initial transmissivity in each simulation was set at 1000 m^2/d, and the initial specific yield was 0.1%. In the first model the transmissivity and storage stayed constant throughout the test, in the second the transmissivity reduced linearly with depth. In the third simulation the transmissivity reduced non-linearly with depth, and in the fourth transmissivity reduced non-linearly and storage reduced linearly.

The simulations were run and the calculated heads were extracted for various distances from the pumping well to produce modelled hydrographs. These were then analysed using a discrete Cooper-Jacob method to try to determine the variation of aquifer properties with depth used in each model from the hydrographs alone.

This method works by calculating the gradient between each successive pair of points in the hydrograph, and calculates a transmissivity based on this gradient using the Cooper-Jacob method. Each value of transmissivity is associated with the level of drawdown of the pair of points. By calculating the difference in transmissivity between successive transmissivity values, and looking at the difference in drawdown, it is possible to make an estimate of the hydraulic conductivity in that drawdown interval.

This method is not very consistent with the assumptions used to derive the Cooper-Jacob method (the models do not represent infinite, confined aquifers), but the values of hydraulic conductivity estimated from the method produce a very good match to the values used to define the model (see Figure C.1), although only after a time sufficient for u (= $r^2S/4Tt$) to be very small (~5 x 10^{-5}).

Comparison of Cooper-Jacob derived hydraulic conductivities from three different pumping test model runs (const T, const K, VKD), constant storage of 1%, observation point 5 m from pumping well.



WATER MANAGEMENT CONSULTANTS

Figure C.1 Discrete Cooper-Jacob analysis of the results of three pumping test models