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The variation of hydraulic conductivity with depth in the object-oriented groundwater model ZOOMQ3D

National Groundwater and Contaminated Land Centre

September 2002

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Object-oriented regional groundwater model ZOOMQ3D
(variation of hydraulic conductivity with depth)

The variation of hydraulic conductivity with depth in the object-oriented groundwater model ZOOMQ3D

Groundwater Systems and Water Quality

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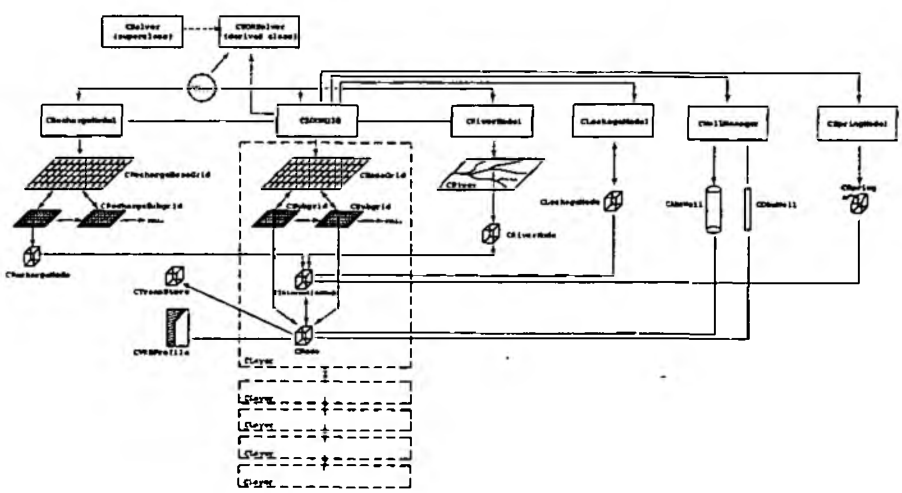
Technical Report NC/01/38/1



BRITISH GEOLOGICAL SURVEY
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ENVIRONMENT AGENCY
National Groundwater & Contaminated Land Centre
Technical Report NC/01/38/1

The variation of hydraulic conductivity with depth in the object-oriented groundwater model ZOOMQ3D

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This report is the result of a study jointly funded by the British Geological Survey's National Groundwater Survey and the Environment Agency's National R&D programme in collaboration with The University of Birmingham.

Environment Agency Dissemination status
Internal: Release to Regions
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Project No. NC/01/38

Statement of use
This document describes the development of the regional groundwater modelling code, ZOOMQ3D.

Cover illustration
ZOOMQ3D object framework

Bibliographic Reference
Jackson, C.R., 2002. The variation of hydraulic conductivity with depth in the object-oriented groundwater model ZOOMQ3D
British Geological Survey Commissioned Report No. CR/02/152N

ISBN **1 85705 988 3**

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National Groundwater & Contaminated Land Centre, Solihull 2002
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Acknowledgements

This work has been undertaken as part of a continuing tripartite collaboration between Dr A. Spink of The University of Birmingham, the Environment Agency, represented by S. Fletcher and P. Hulme of the National Groundwater and Contaminated Land Centre and The British Geological Survey. The project has been co-funded by the Environment Agency's National Groundwater and Contaminated Land Centre and BGS. The assistance of Paul Hulme of the Environment Agency and Adam Taylor of Water Management Consultants, who both worked on the implementation of VKD in MODFLOW, has been greatly appreciated.

Contents

FIGURES

TABLES

Summary

This report documents the implementation of the variation of hydraulic conductivity with depth within layers of the object-oriented regional groundwater model ZOOMQ3D. This representation of the vertical variation of hydraulic conductivity provides an alternative to the development of multi-layer models, in which individual layers are characterised by uniform horizontal hydraulic conductivity in the vertical direction.

The approach has been developed to enable the more accurate description of the variation the hydraulic conductivity in limestone, and particularly Chalk aquifers, in which higher hydraulic conductivity values are often associated with the zone of fluctuation of the water table. The method circumvents numerical difficulties that are related to the de-watering of layers in multi-layer models.

The incorporation of the vertical variation of hydraulic conductivity with depth (VKD) mechanism has been rapidly incorporated into ZOOMQ3D due to the flexibility of the object-framework. The model has been rigorously tested by its comparison with a modified MODFLOW model (Environment Agency, 1999) in which VKD has also been implemented.

1 Background

The accurate simulation of flow in Chalk aquifers requires the careful consideration of the conceptual model of Chalk groundwater systems. It is then necessary to translate the conceptual model into a numerical model accurately if groundwater flow in the Chalk is to be simulated satisfactorily. An important component of the conceptualisation of Chalk groundwater flow is the description of the aquifer's hydraulic properties and in particular the representation of the variation of hydraulic conductivity. For example, modelling of Chalk aquifers has shown that it can be difficult to simulate river-aquifer interaction, spring flow and the response of groundwater heads to recharge correctly if the vertical variation of hydraulic conductivity is not represented properly.

Typically, Chalk aquifers are highly permeable low storage systems, which respond quickly to recharge. The majority of groundwater flow occurs in the upper part of chalk aquifers, where dissolution of the chalk has enlarged fractures and hydraulic conductivity generally increases towards river valleys and decreases with depth. Higher hydraulic conductivities near the water table promote good hydraulic connection between rivers and the aquifer and the outflow from springs can also be extremely high. A particular feature of chalk catchments is that the head of ephemeral streams can move several kilometres seasonally because of the relationship between discharge, groundwater head and hydraulic conductivity.

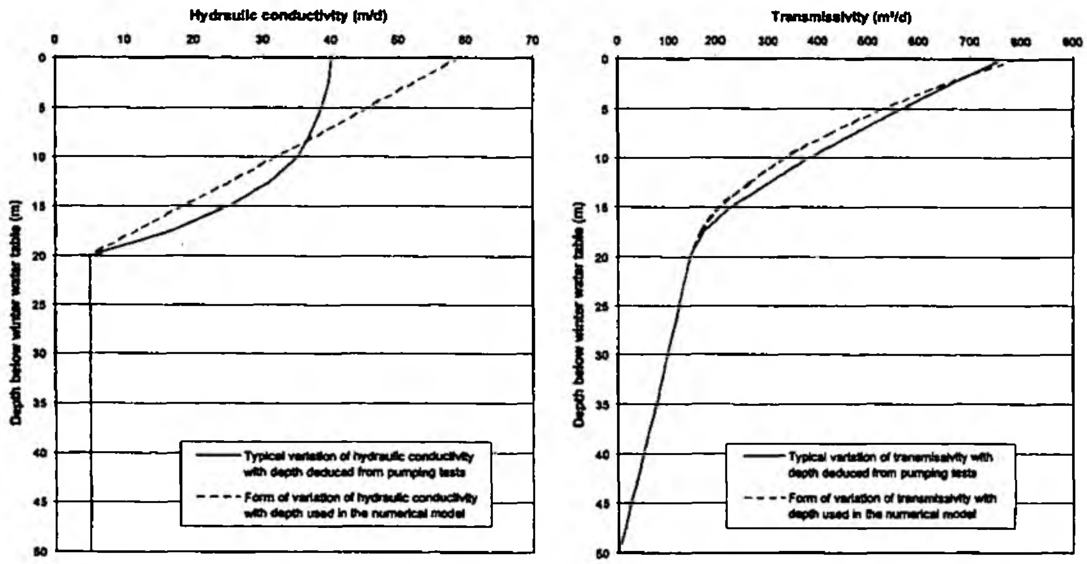


Figure 1 Conceptual diagram of the relationship between hydraulic conductivity and depth, after Environment Agency (1999).

The variation in hydraulic conductivity with depth can be incorporated in a groundwater model with the use of multiple layers. However, this can cause numerical difficulties when layers de-water and re-wet. Another approach is to use a single layer but to allow hydraulic conductivity to vary within it. That is, to calculate transmissivity by integrating the hydraulic conductivity over the layer's saturated thickness, as illustrated in Figure 1. This method has been implemented in MODFLOW (McDonald and Harbaugh, 1988) by the Environment Agency (Environment Agency, 1999; Taylor et al., 2001) in order to improve the simulation of chalk behaviour in a number of regional groundwater models. This report describes the implementation of the same variation of hydraulic conductivity with depth (VKD) mechanism in the object-oriented regional groundwater model, ZOOMQ3D.

2 Methodology

The implementation of VKD in ZOOMQ3D is based on two principal concepts. These are the definition of VKD *profiles* and VKD *schemes*. These two terms are used to describe both the incorporation of the mechanism in the model code and the input of data to the model.

2.1 VKD PROFILES

A VKD *profile* describes the change in hydraulic conductivity with depth at a particular point in the aquifer. An example VKD profile is shown in Figure 2. Currently, VKD profiles represent the variation in hydraulic conductivity with elevation using a relatively simple method. Profiles are defined by two sections. In the lower section, between Z_{BOTTOM} and Z_P in Figure 2, hydraulic conductivity is constant. In the upper section, between Z_P and Z_{TOP}, hydraulic conductivity increases linearly with elevation. Because different values of hydraulic conductivity can be specified in the two orthogonal horizontal directions (x and y), six values are required to parameterise an individual profile:

i. The elevation of the base of the profile, Z_{BOTTOM}.

ii. The elevation of the top of the profile, Z_{TOP}.

iii. The elevation of the point of inflection, Z_P.

iv. The hydraulic conductivity in the x direction, K_x^*, below Z_P.

v. The hydraulic conductivity in the y direction, K_y^*, below Z_P.

vi. The gradient of the profile above Z_P, VKDGrad. This is equal to the increase in hydraulic conductivity per metre rise in elevation.

The value of the VKDGrad parameter may be either negative, zero or positive. Consequently, in addition to an increase in hydraulic conductivity with depth above Z_P, hydraulic conductivity can be specified to decrease or remain constant. VKDGrad is given by:

$$\text{VKDGrad} = \frac{dK_x}{dZ} = \frac{dK_y}{dZ}$$

To calculate transmissivity the following equations are used:

$$T_x = K_x^*(h - Z_{BOTTOM}) + 0.5\text{VKDGrad}\cdot(h - Z_P)^2$$

$$T_y = K_y^*(h - Z_{BOTTOM}) + 0.5\text{VKDGrad}\cdot(h - Z_P)^2$$

for $h > Z_P$, and,

$$T_x = K_x^*(h - Z_{BOTTOM})$$

$$T_y = K_y^*(h - Z_{BOTTOM})$$

for $h \le Z_P$, where h is the water table elevation.

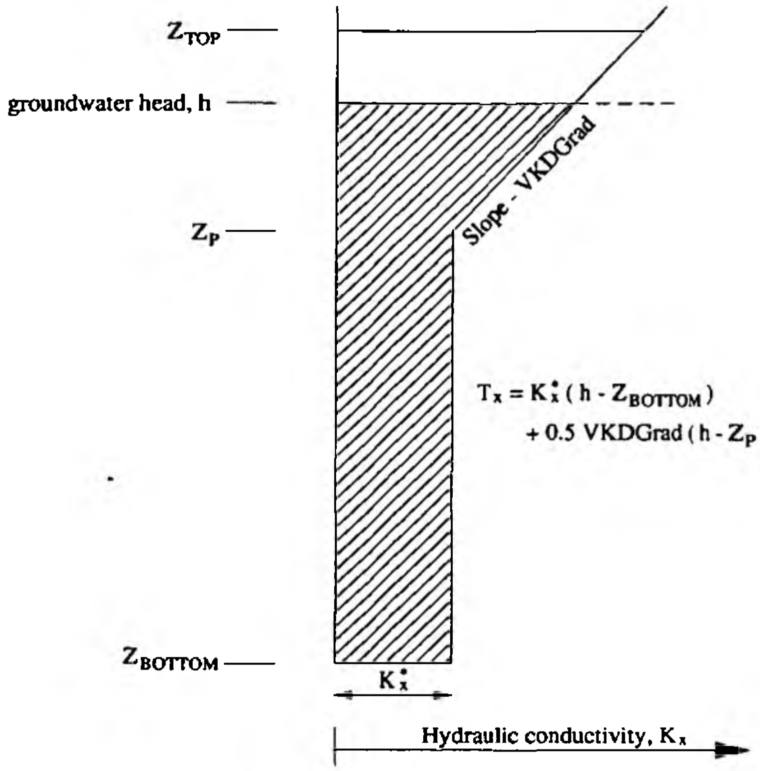


Figure 2 Parameters used to define VKD profiles in ZOOMQ3D

The implementation of the VKD mechanism in MODFLOW (Environment Agency, 1999) differs slightly from the method employed in ZOOMQ3D in that the MODFLOW model does not use the gradient term VKDGrad. Instead *hydraulic conductivity gradient factors*, FACX and FACY are used. These are related to the gradient of the profile above Z_P by the following equations:

$$\frac{dK_x}{dZ} = FACX \cdot K_x^*, \qquad \frac{dK_y}{dZ} = FACY \cdot K_y^*$$

The modified MODFLOW model uses a factor for each direction, however, this facility has not been included in ZOOMQ3D. In MODFLOW these factors can be calculated automatically using a VKD profile parameterisation procedure. This procedure is based on a steady-state simulation in which transmissivity is specified. The resulting simulated groundwater heads, the specified transmissivities and the VKD profile elevations are then used to calculate the hydraulic conductivities, K_x^* and K_y^* and the hydraulic conductivity gradient factors, FACX and FACY, for each VKD profile in the model. This procedure is incorporated in the MODFLOW model to provide a method to obtain appropriate sets of starting conditions for time-variant model simulations. However, application of the model by the Environment Agency has shown that stable steady-state starting conditions can generally be simulated without performing this prior parameterisation procedure (Hulme and Taylor, personal communication, January 2002). Consequently, the automatic VKD profile parameterisation procedure has not been incorporated in ZOOMQ3D, which has promoted the use of only one unidirectional value of VKDGrad for simplicity. Furthermore, only one value is defined for VKDGrad and Z_P because it is considered that further hydrogeological investigations are required to justify the need for the direction dependence of these parameters. This should involve a more detailed review of the MODFLOW model modified by the Environment Agency (1999) and include an examination of the application of this model to real aquifers.

2.2 VKD SCHEMES

A VKD *scheme* defines the number of VKD profiles in the vertical, at a horizontal point, and the number of model layers that each profile in the scheme crosses. That is, a scheme simply stores how VKD profiles are arranged in the vertical at a horizontal nodal location. In the current implementation of VKD in MODFLOW (Environment Agency, 1999) VKD profiles can only be defined in the top layer of a model. Furthermore they are restricted to being active at purely *unconfined* nodes. They cannot be defined at nodes which convert between unconfined and confined conditions. The implementation in ZOOMQ3D is not restricted in this way. VKD profiles can be specified in any layer and at both unconfined and convertible nodes. The following points describe the use of VKD schemes.

i. A VKD scheme defines the number of VKD profiles in the vertical at a horizontal nodal location.

ii. The number of VKD profiles in a scheme must be in the range zero to the number of numerical layers in the model.

iii. Within a scheme, a single VKD profile can be defined to cross/represent only one or more than one model layers. The scheme defines which layers each VKD profile represents.

iv. VKD profiles can be defined to cross layers of *confined* nodes. The confined nodes are not connected to the VKD profile and do not calculate their transmissivity by interrogating the profile.

v. A different scheme can be defined at each horizontal nodal location of the model.

vi. The same scheme can be applied at multiple horizontal nodal locations.

Figure 3 shows a number of examples of different VKD schemes in a model with four layers. Consequently, the maximum number of profiles in the vertical is four. These examples are not intended to be physically realistic but rather meant to illustrate the flexibility of the method. This level of flexibility has been included with regard to the possible future development of the method. It may be the case that more complex but realistic variations of hydraulic conductivity with depth are defined at a later stage of model development. The model can easily be modified to incorporate such VKD profiles.

The representation of the variation of hydraulic conductivity with depth using schemes and profiles, as shown in Figure 3, is very similar to its implementation in the model code. One additional *class*, the template for an object, has been added to the framework on which ZOOMQ3D is based. This class encapsulates all the data and functionality required by the model to implement the VKD mechanism. The modification of the model framework is described next.

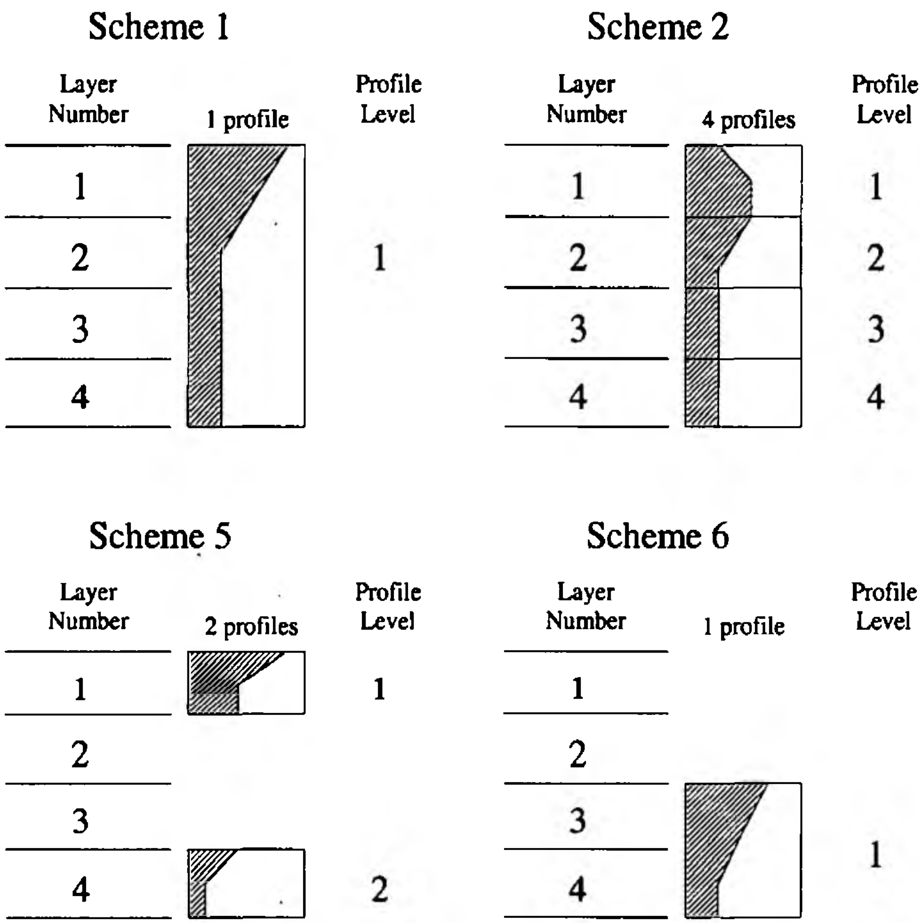
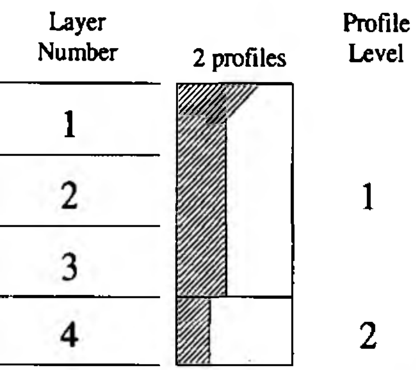
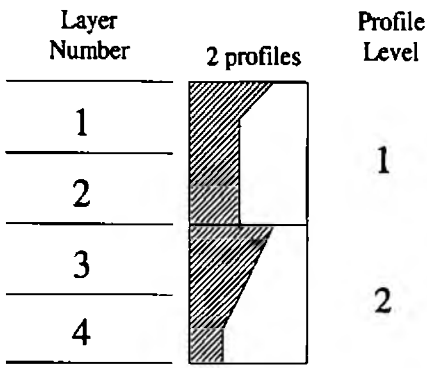


Figure 3 Specification of VKD schemes in ZOOMQ3D

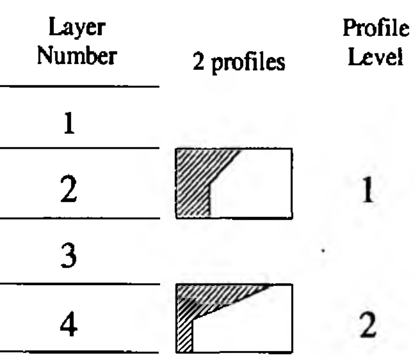
Scheme 3



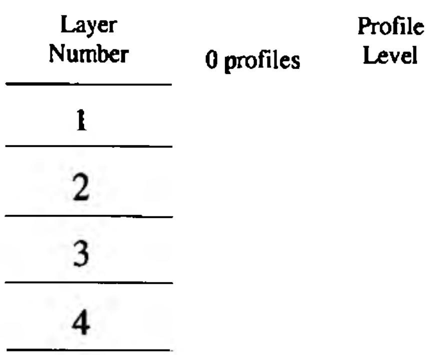
Scheme 4



Scheme 7



Scheme 8



3 The implementation of VKD in the object framework

Figures 5 and 6 show the framework of classes on which ZOOMQ3D is based before and after the implementation of the VKD mechanism, respectively. Only one *class*, the template for an object, has been added to the framework. This is the CVKDProfile class. Each object, or instance of this class, stores four of the six parameters defined in Figure 2. These are:

i. The elevation of the point of inflection, Z_P.

ii. The hydraulic conductivity in the x direction, K_x^*, below Z_P.

iii. The hydraulic conductivity in the y direction, K_y^*, below Z_P.

iv. The gradient of the profile, VKDGrad, above Z_P.

In addition to these parameters describing the variation of hydraulic conductivity with depth each CVKDProfile object contains three additional parameters. These are:

i. The number of the top layer represented by the profile.

ii. The number of the bottom layer represented by the profile.

iii. A *pointer* to the CVKDProfile object below. A pointer is a programming term and may be thought of simply as a connection between objects (or *type* variables, i.e. integers) via which information can be passed.

The final modification to the model framework is the addition of a pointer variable to the CConvertibleNode class. To explain this a brief description of the objects used to differentiate between unconfined and confined conditions must be presented.

Unconfined behaviour is incorporated in the model using the object-oriented concept of *inheritance*. Three types of node objects are defined in the object framework: CNode, CConfinedNode and CConvertibleNode as shown in Figure 4. The objects of type CConfinedNode and CConvertibleNode are derived from the base class CNode. Objects are never created directly from the CNode class. Instead, only objects of type CConfinedNode and CConvertibleNode are created. Only the base class, CNode, is represented in Figure 5 and 6, which shows the model object framework.

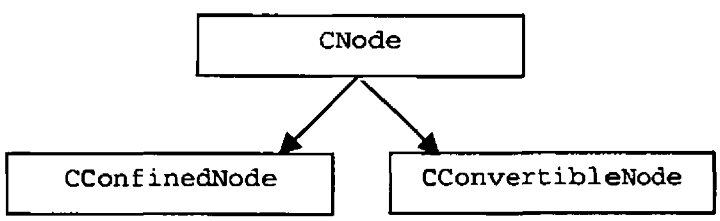


Figure 4 Use of inheritance to define confined and unconfined aquifer conditions

In CConfinedNode objects the transmissivity is always constant as it is independent of the saturated thickness. CConvertibleNode objects contain the functionality to calculate transmissivity based on the difference between the groundwater head and the elevation of the base of the node. It is to this class of objects that a pointer is added in order to implement VKD. This additional pointer variable connects CConvertibleNode objects of the model grid with CVKDProfile objects. Using this connection a CConvertibleNode object can request that its CVKDProfile object integrates hydraulic conductivity over the node's saturated thickness and returns to it the transmissivity in the x and y-directions.

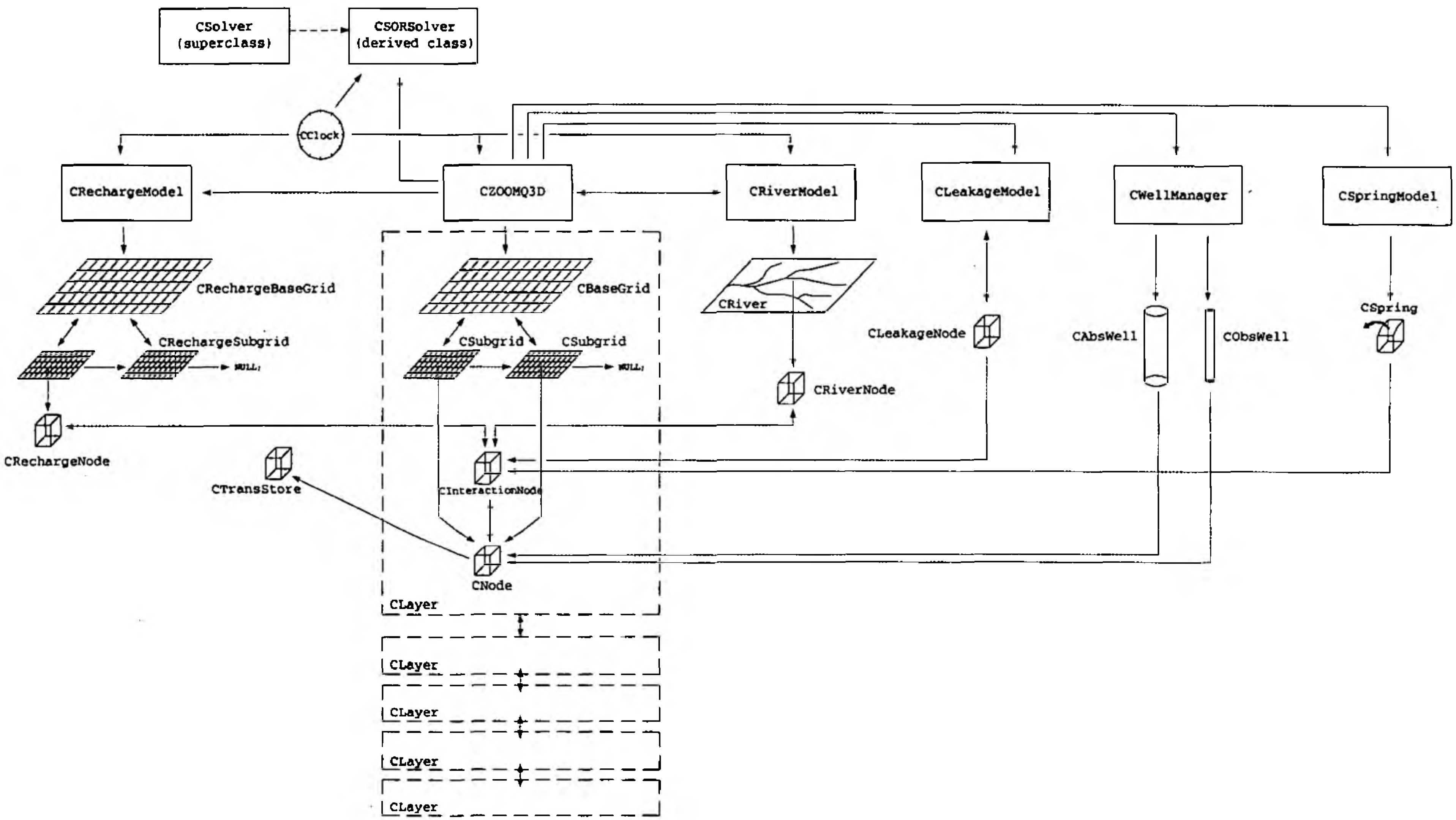


Figure 5 ZOOMQ3D object framework prior to the incorporation of VKD

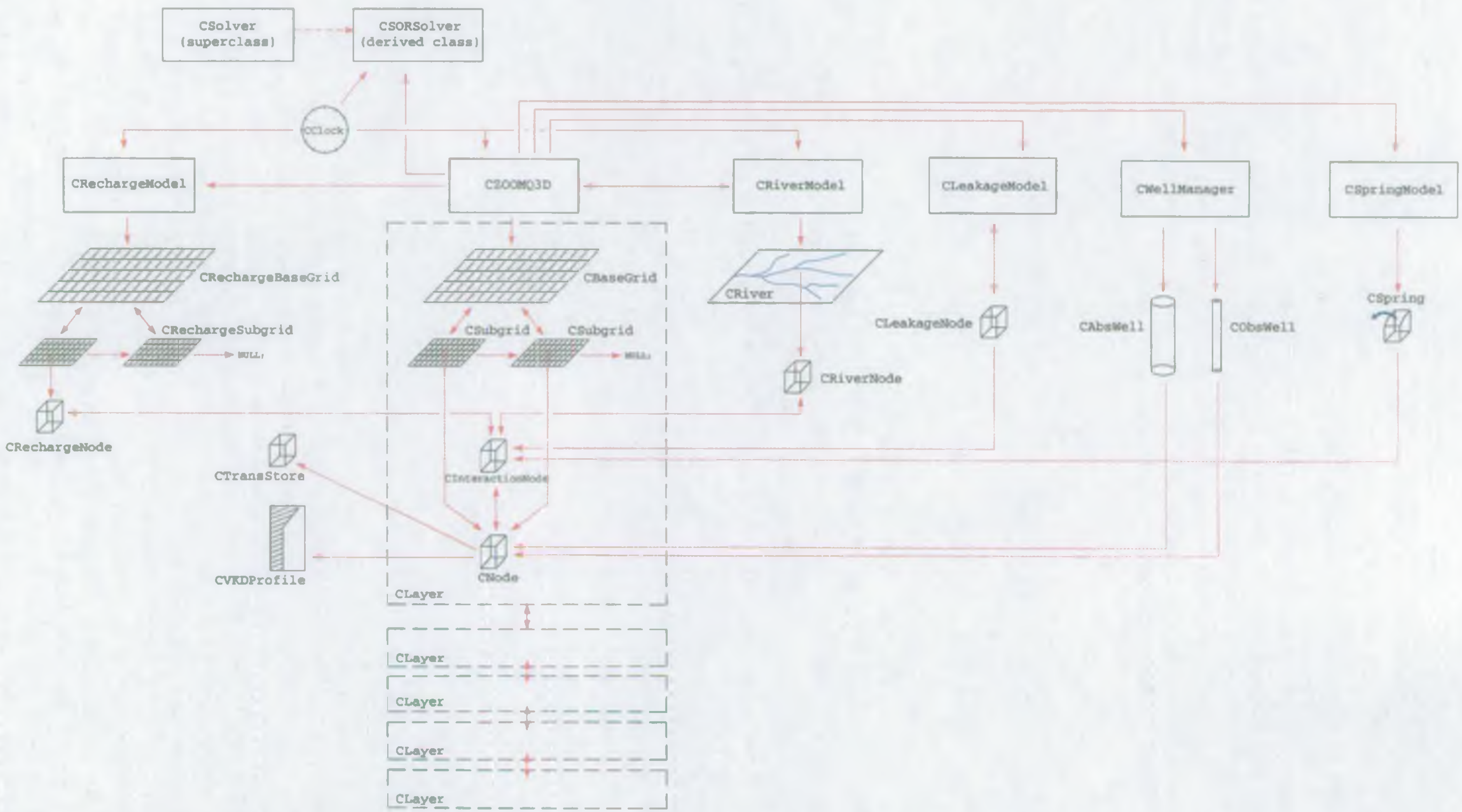


Figure 6 ZOOMQ3D object framework after the incorporation of VKD

4 Data input

4.1 VKD SCHEME DATA FILES

Input data to the model can be separated into two categories. First information must be read to define the number and types of schemes in the model. Second, data must be entered to define the VKD profiles at each horizontal nodal location of the model mesh. Examples data files are presented for a relatively simple model in Appendix 2. Two text input files are required to enter VKD scheme information into the model: "vkd.cod" and "vkd.map". The first of these ASCII files, "vkd.cod" contains the following lines of data:

$$
\begin{array}{l}
NS \\
NP_1 \;,\; I^1_{TOP} \;,\; I^1_{BOT} \;,\; I^2_{TOP} \;,\; I^2_{BOT} \;,\; \ldots\ldots\ldots\ldots\ldots \;,\; I^{NP_1}_{TOP} \;,\; I^{NP_1}_{BOT} \\
NP_2 \;,\; I^1_{TOP} \;,\; I^1_{BOT} \;,\; I^2_{TOP} \;,\; I^2_{BOT} \;,\; \ldots\ldots\ldots\ldots\ldots \;,\; I^{NP_2}_{TOP} \;,\; I^{NP_2}_{BOT} \\
\vdots \qquad \vdots \qquad \vdots \qquad \vdots \qquad \vdots \qquad\qquad\qquad\quad \vdots \qquad \vdots \\
NP_{NS} \;,\; I^1_{TOP} \;,\; I^1_{BOT} \;,\; I^2_{TOP} \;,\; I^2_{BOT} \;,\; \ldots\ldots\ldots\ldots\ldots \;,\; I^{NP_{NS}}_{TOP} \;,\; I^{NP_{NS}}_{BOT}
\end{array}
$$

where

NS is the number of schemes in the model.

NP_i is the number of profiles in the i^{th} scheme ($i = 1$ to NS).

I^j_{TOP} is the number of the top layer in the j^{th} profile in the scheme ($j = 1$ to NP_i).

I^j_{BOT} is the number of the bottom layer in the j^{th} profile in the scheme ($j = 1$ to NP_i).

Therefore to define the eight schemes shown in Figure 3 "vkd.cod" would contain the following lines of data:

```
8
1  1 4
4  1 1  2 2  3 3  4 4
2  1 3  4 4
2  1 2  3 4
2  1 1  4 4
1  3 4
2  2 2  4 4
0
```

4.2 VKD PROFILE DATA FILES

Once the schemes have been defined in the vertical, that is, the profiles have been specified within each scheme, information relating to the distribution of the schemes in the horizontal must be entered. This is performed using the text file "vkd.map", which contains a map of the model mesh. For example consider the file shown in Figure 7, which represents the square mesh that is also shown in the figure. At each node of the mesh a character is specified. Each letter of the alphabet corresponds to a VKD scheme defined in "vkd.cod". Fifty-two letters, and therefore schemes, are allowed which are specified in the order a-z and then A-Z. Letter 'a' corresponds to the first scheme, 'b' to the second and 'z' to the twenty-sixth scheme. Letter 'A' corresponds to the twenty-seventh scheme, 'B' to the twenty-eighth and 'Z' to the fifty-second scheme. Figure 7 shows the example of a map file, which is used to distribute the VKD schemes defined in Figure 3 over the model domain. VKD profiles are not created at the horizontal nodal locations where an appropriate letter is not specified i.e. in this example where the character is not in the range 'a' to 'h'. At these points horizontal conductivity is uniform in the vertical direction within each layer. Again this example is not intended to be physically realistic but rather is used to illustrate the flexibility of the method.

```
Map of VKD schemes
-----abbbcc
----abbccdd
---abccdddd
--abccddeee
--abcdddeef
-abcddeefff
abcddeeffgg
bcddeeffggh
cddeeffghhh
cddeeffghhh
cdeefgghhhh
```

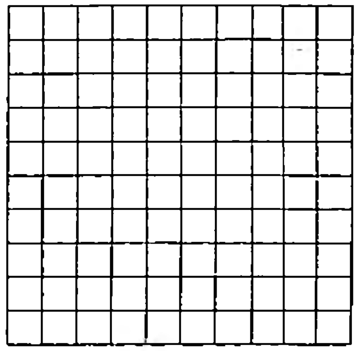


Figure 7 VKD scheme map file and associated model grid

After the VKD schemes and profiles have been set up at each horizontal nodal location parameter values have to be read for each of the VKD profiles. At horizontal nodal locations represented by the letter 'a', in this example, data for only one profile is required. But at nodal locations represented by the letter 'b' data for four profiles must be read in. Four types of information are required for each VKD profile:

i. The hydraulic conductivity in the x direction, K_x^*, below Z_P.

ii. The hydraulic conductivity in the y direction, K_y^*, below Z_P.

iii. The gradient of the profile, VKDGrad, above Z_P.

iv. The elevation of the point of inflection, Z_P.

A set of four pairs of data files is provided for each *profile level*. As shown in Figure 3, profiles can be on the same level but represent/cross different model layers. Reiterating, VKD profile data is input on a profile level by profile level basis and not on a model layer by model layer basis. Eight data files are required for each profile level. An example set of eight files for the profiles on level 1 is:

```
vkdkx01.cod       vkdkx01.map
vkdky01.cod       vkdky01.map
vkdgrad01.cod     vkdgrad01.map
vkdzp01.cod       vkdzp01.map
```

The number in the file name relates to the profile level. Hence, three additional sets of files are required with names containing 02, 03 and 04 instead of 01. This is because, in this example, the maximum number of profiles in the vertical is four. The part of the file name preceding the number can be defined by the user, which simplifies the management of different data sets.

Each of these pairs of code (.cod) and map (.map) files is used to input the values of one of the VKD profile parameters on a particular profile level. For example, considering the first pair, vkdkx01.cod and vkdkx01.map for which examples are shown in Figure 8. The first line of each file is a comment line. On the second line of the code file the standard hydraulic conductivity, $\overline{K}_x^*$, and the number of codes or factors, N_c, is defined. For each of the N_c codes one multiplier is then entered per line. The first factor corresponds to the letter 'a', the second to 'b' etc. Consequently, where the letter 'a' is defined in the map file the hydraulic conductivity, K_x^*, of the profile will be assigned a value of 17.0 (10.0 × 1.7). Where the letter 'b' is specified in the map file the hydraulic conductivity, K_x^*, of the profile will be assigned a value of 23.0 (10.0 × 2.3). This method of data entry is identical for the three remaining sets of information required by each profile on each level: K_y^*, VKDGrad and Z_P.

Code file	**Map file**
VKDKx code data	Map for VKDKx parameter on profile level 1
10.0 2	-----aaaaaa
1.7	----aaaaaaa
2.3	---aaaaaabb
	--aaaaaabbb
	--aaaaaabbb
	-aaaaabbbbb
	aaaaabbbbbb
	aaaabbbbbbb
	aaabbbbbbbb
	aaabbbbbbbb
	aabbbbbbbbb

Figure 8 Example ASCII code file (vkdkx01.cod) and map file (vkdkx01.cod)

5 Simulation of phreatic aquifers in ZOOMQ3D

Prior to the testing of the implementation of VKD in ZOOMQ3D it is necessary to review the technique by which unconfined aquifers are simulated in the model. This is required to explain the differences observed between the models used in the validation of the VKD mechanism.

Unconfined behaviour is represented as a cyclical process within ZOOMQ3D. The finite difference equations are solved repeatedly during *each* time-step. Each unconfined node calculates its transmissivity at the beginning of the time-step based on the groundwater head. A solution to the finite difference equations is then computed. The transmissivity is subsequently recalculated using the new heads. An average is then taken of the pre and post-solution transmissivities at each unconfined node. A new solution to the finite difference equations is computed again using the average of the two transmissivity values. This cyclical process continues until the transmissivity variation over a cycle is negligible at all the unconfined nodes.

The test for convergence within the repetitive cycle is based on a maximum nodal flow imbalance. At the end of a cycle, after the solution has been computed and the averages of the transmissivities have been calculated, nodal flow imbalances are examined. Nodal flow balances are calculated using the heads computed at the end of the i^{th} cycle (based on the transmissivities at the beginning of the i^{th} cycle) and the average transmissivities calculated at the end of the i^{th} cycle. If the maximum flow imbalance is below a small user defined value then the difference between the pre and post-solution transmissivities is small. The solution then progresses to the *next* time-step. This process is illustrated in Figure 9.

This method of simulating unconfined aquifers differs from that used in MODFLOW, which is used in this work as a benchmark for the modified ZOOMQ3D code. In the version of MODFLOW used here, which has been modified to incorporate the VKD mechanism (Environment Agency, 1999), the transmissivity can either be calculated once at the start of the time-step using the current heads or it can be updated after each *iteration* of the solution procedure. The first of these two methods can be reproduced in ZOOMQ3D by stopping the transmissivity cycling within a time-step. However, the coefficients of the finite difference equations cannot be updated during the iterations of the solution procedure. This is because in ZOOMQ3D the system of simultaneous finite difference equations cannot be changed whilst they are being solved.

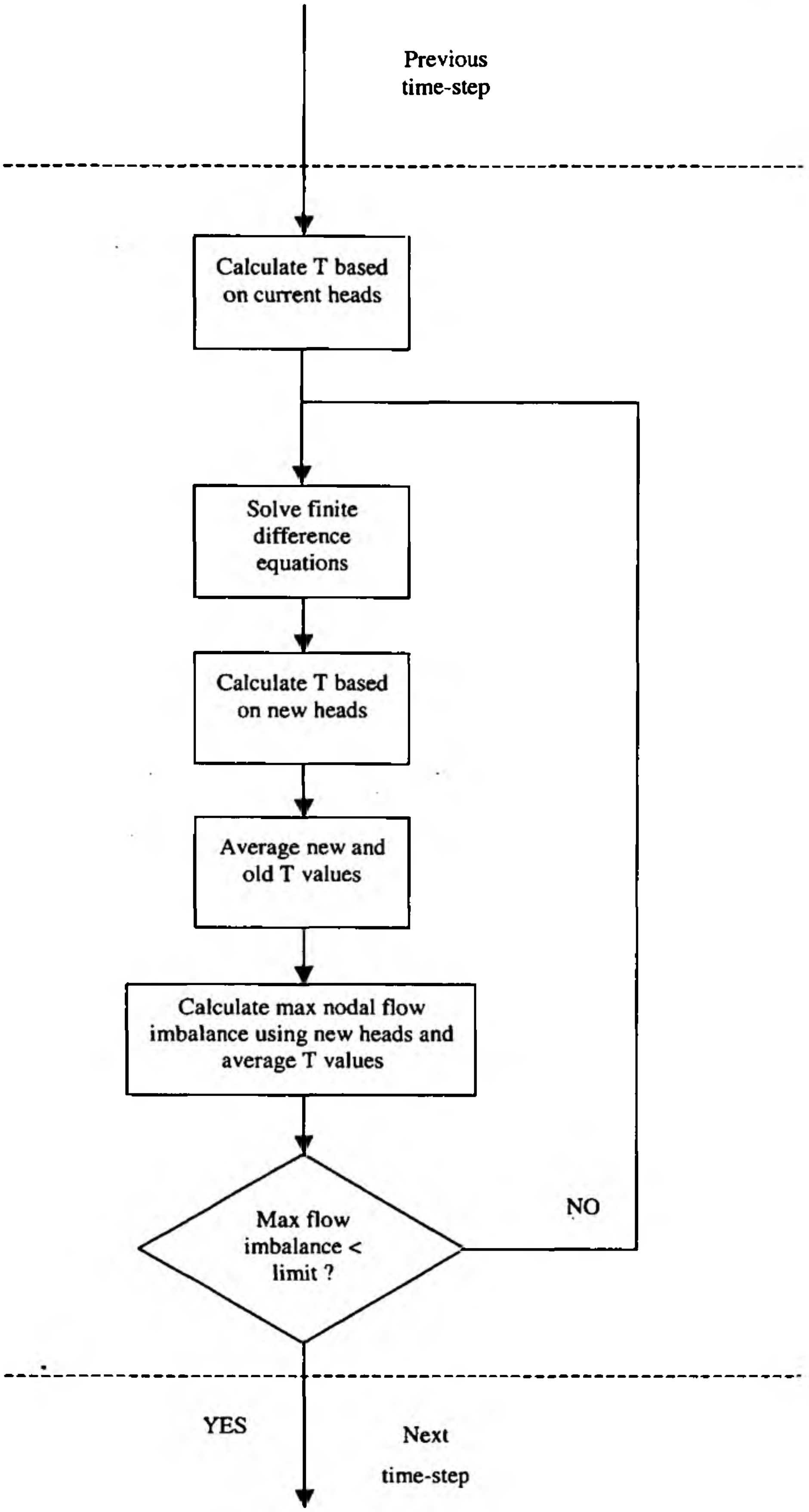


Figure 9 Flowchart of the cyclical transmissivity updating process when simulating unconfined aquifers

6 Model testing

The validation of the incorporation of VKD in ZOOMQ3D is performed through comparison of the model with the modified MODFLOW model (Environment Agency, 1999). The modified MODFLOW code has been benchmarked against another groundwater model code developed by The University of Birmingham (Environment Agency, 1999). The example model used to benchmark the MODFLOW code against the Birmingham code is also used here to compare ZOOMQ3D with MODFLOW. The development and testing of the implementation of VKD in MODFLOW is described in detail in Environment Agency (1999).

The model used to compare ZOOMQ3D and MODFLOW is shown in Figure 10. The grid is eleven kilometres long in the x-direction and ten kilometres long in the y direction and is composed of a regular 500 m square mesh. All boundaries are impermeable and recharge is distributed uniformly over the aquifer. A line of head dependent leakage nodes is specified between co-ordinates (1000 m, 0 m) and (1000 m, 10000 m). The elevation of each of these leakage nodes is set at 101 m above the base of the aquifer. Outflow from the leakage nodes is dependent on the difference between the groundwater head and its elevation and is given by:

$$Q = C \cdot (h - z_L)$$

where

Q is the outflow from the leakage node (m^3/day),

h is the groundwater head (m),

Z_L is the elevation of the leakage node (m) and,

C is the leakage coefficient (m^2/day).

The leakage coefficient is specified as 5000 m^2/day for each of the leakage nodes in the test model.

An abstraction well is located at co-ordinate (3500 m, 4500 m) and pumps at a constant rate. This is near to a river, which runs from (9500 m, 2500 m) to (1500 m, 8000 m) downstream. The river is composed of seventeen nodes. At its upstream end the river bed is 130 m above the base of the aquifer and at its downstream end the elevation of the river bed is 101.75 m. At co-ordinate (8500 m, 3500 m) a constant rate anthropogenic inflow to the river is specified. The model simulates the flow in the river, which depends on gains from the aquifer where it is influent and losses along effluent reaches. Note that there is a slight difference in terminology between ZOOMQ3D and MODFLOW. ZOOMQ3D *rivers* are equivalent to MODFLOW *streams*. Along these model features river flow accounting is performed. ZOOMQ3D *leakage nodes* are equivalent to MODFLOW *river nodes*. These nodes are unconnected and consequently they cannot be used to generate flow accretion profiles. In this report ZOOMQ3D terminology is adopted.

A further point to note is that the model shown Figure 10 is *grid-centred* model. ZOOMQ3D is grid-centred, however, MODFLOW is *block-centred*. The boundaries of the MODFLOW model are actually half a mesh interval (250 m) further outside the boundary shown in Figure 10. At the blocks on the boundary of the MODFLOW model, hydraulic conductivity, storage and recharge are modified in order to maintain its equivalence with the ZOOMQ3D model and the earlier grid centred Birmingham model. These adjustments are described in detail in Environment Agency (1999).

The values of the VKD parameters are presented in Appendix 1. In summary the model represents a section of a river valley and its interfluve. Towards the left of the model domain, along the line of leakage nodes, the aquifer is thicker and hydraulic conductivity is greater. In this region, representing a conceptual Chalk river valley, transmissivity is approximately

2000 m^2/day. The aquifer thins and hydraulic conductivity reduces towards the right hand boundary. On the right hand boundary transmissivity is approximately 50 m^2/day. Figure 11 illustrates the variation of these aquifer parameters across the centre of the model from left to right. The simulated steady-state position of the water table is also plotted in Figure 11. This simulation is described subsequently.

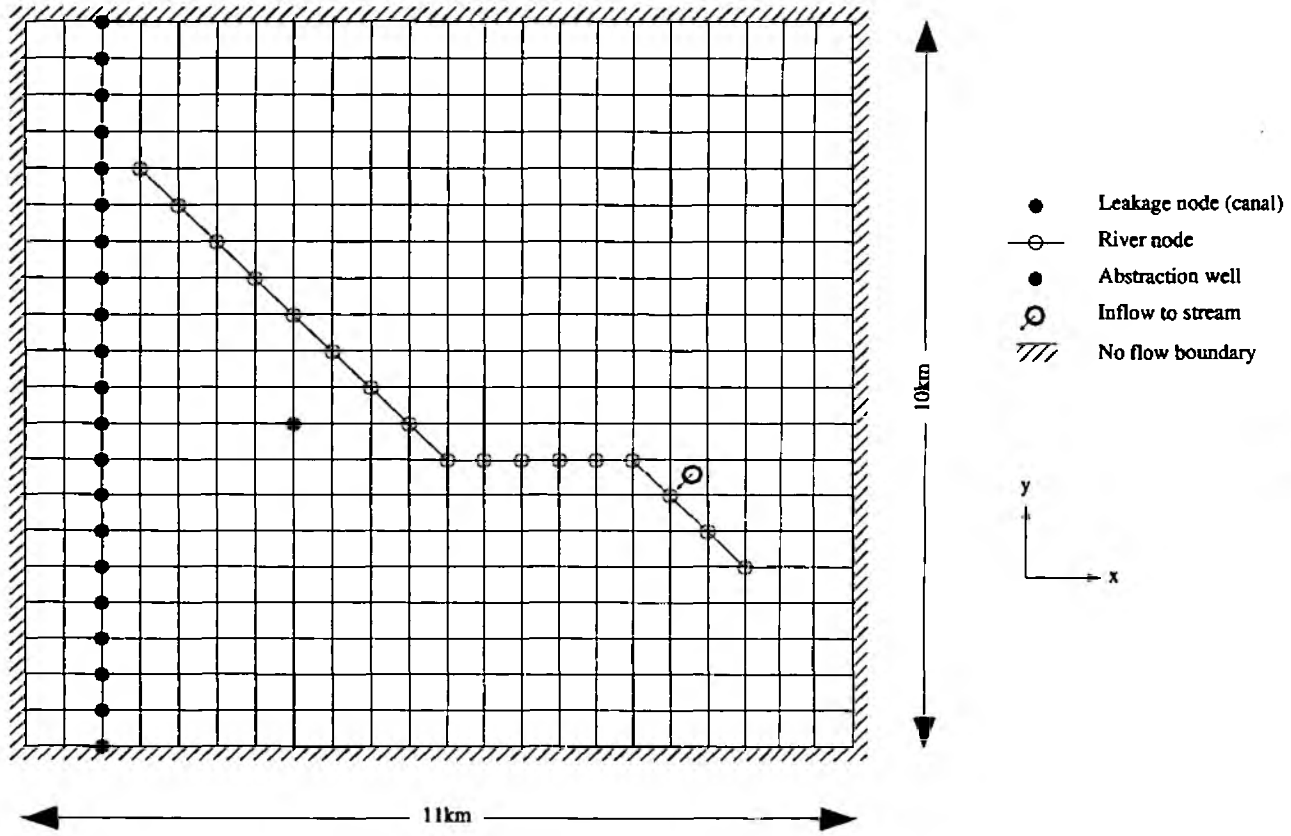


Figure 10 Model used for comparison of ZOOMQ3D with MODFLOW

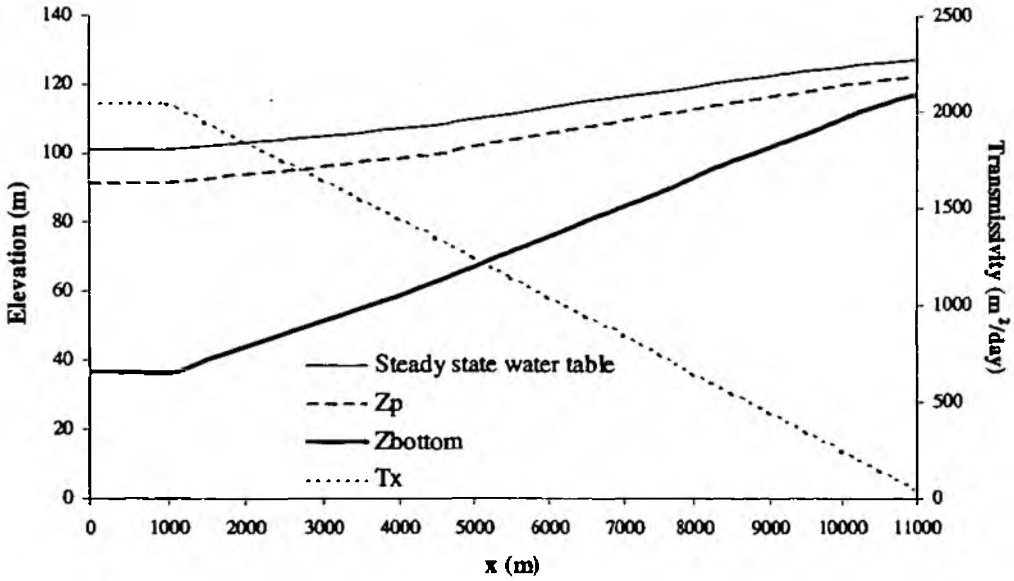


Figure 11 Variation of VKD parameters and transmissivity across the centre of the test model from left to right (y=5000 m)

6.1 ACCEPTANCE CRITERIA

A set of acceptance criteria were defined for the previous comparison of the modified MODFLOW model and the Birmingham model (Environment Agency, 1999). These criteria are adopted here for the comparison of the test ZOOMQ3D and MODFLOW models. The acceptance criteria are as follows:

1. The difference in head between the ZOOMQ3D model and the MODFLOW model is no greater than 0.5% of the range of heads (maximum head minus minimum head) where the maximum and minimum heads are taken from all nodes for the entire simulation. Thus:

   $$\left(H_{ZOOMQ3D} - H_{MODFLOW}\right) / \left(H^{MAX}_{MODFLOW} - H^{MIN}_{MODFLOW}\right) < 0.5\%$$

2. The hydrograph of transmissivity at any node must be within 1% of the value from the MODFLOW code. Thus:

   $$\left(T_{ZOOMQ3D} - T_{MODFLOW}\right) / T_{MODFLOW} < 1\%$$

3. The flow accretion for the ephemeral river must be within 2% of the value produced by the MODFLOW code. That is, the difference between the flow into or out of an ephemeral river node calculated by the ZOOMQ3D and MODFLOW code must be less than 2% of the maximum accreted flow in the river at that time.

4. The total inflows and outflows from ZOOMQ3D are within 0.5% of those from the MODFLOW code. That is, the difference in the global flow balance obtained by ZOOMQ3D compared to MODFLOW, for any boundary condition or mechanism (leakage, storage change etc) has to be less than 0.5%.

5. The ZOOMQ3D water balance error at each node does not exceed 0.5% of the total input flow to the node.

The fifth of these acceptance criteria is always satisfied by the ZOOMQ3D model. This is because the model's solution method convergence criterion is defined as a maximum nodal flow imbalance. This maximum flow residual is set to a small value within the following simulations (generally 10^{-8} m^3/day) and consequently nodal water balance errors are very small and less than that defined by acceptance criterion five above.

In the following test simulation the number of times these criteria are not met is cited (as number per simulation). The maximum possible number of failures for each of these criteria is listed in Table 1.

Table 1 List of the theoretical maximum number of failures of each VKD acceptance criterion

Acceptance criterion	Maximum number of failures per time-step
1. Groundwater head	Number of columns of grid × Number of rows
2. Internodal transmissivity	(Number of columns of grid −1) × (Number of rows −1)
3. River flow	Number of river nodes
4. Global flows	Number of global flow balance terms

6.2 TEST 1: STEADY-STATE SIMULATION

A steady-state simulation is run using the model shown in Figure 10. The comparison is made between ZOOMQ3D and MODFLOW as a first test of the implementation of VKD in the code. In this simulation the abstraction well does not pump groundwater from the aquifer. Furthermore, the anthropogenic input to the river is removed from the model. Recharge is applied uniformly over the aquifer at a rate of 0.627 mm/day. The simulated steady-state groundwater head contours are shown in Figure 12. The results of two models are almost identical. The maximum difference in head is 1.4 mm at (11000 m, 2500 m). This is equivalent to only 5.2×10^{-3} % of the variation in groundwater head over the aquifer.

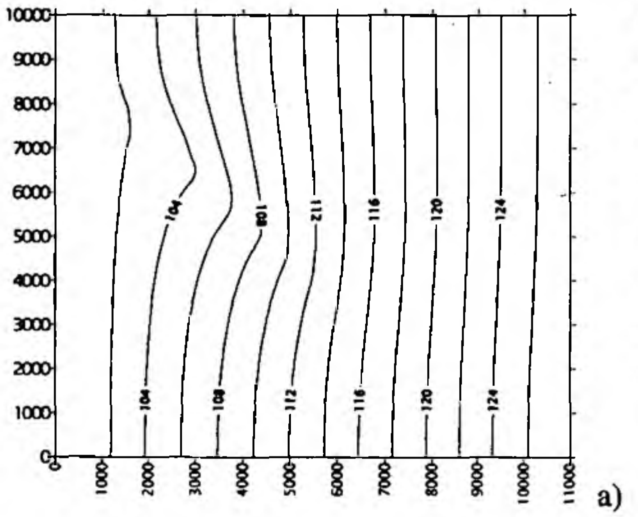


Figure 12 Simulated steady-state groundwater head contours for a) the MODFLOW model and b) the ZOOMQ3D model

To illustrate the level of agreement between the two models in more detail, simulated groundwater heads are listed in Table 2 for the nodes across the centre of the grid from left to right. The maximum difference in head across this section is 0.5 mm. The maximum difference in transmissivity, in both the x and y direction, is 0.61 m^2/day or 0.026 % of the MODFLOW transmissivity at the corresponding node. The difference in river flow between the two models is also negligible. Nodal river flows are listed in Table 3. The eight river nodes at the upstream end of the river are all dry. The maximum difference in flow occurs at the fourth river node upstream and is only 0.08 m^3/day. The global flow balance information output by ZOOMQ3D is listed below.

```
ZOOMQ3D STEADY-STATE GLOBAL FLOW BALANCE
--------------------------------
Total recharge: 68970 m³/d
River 1
  Downstream flow: 20838.1 m³/d
  Anthropogenic input: 0 m³/d
Total leakage out of aquifer: 48131.9 m³/d
Total decrease in aquifer storage: 2.84957e-010 m³/d
GLOBAL FLOW IMBALANCE: 2.99509e-010 m³/d
```

The global flow imbalance is very small, however, the simulation only needs to run for approximately a second to achieve this level of accuracy.

Table 2 Comparison between ZOOMQ3D and MODFLOW groundwater heads (m) and transmissivities (m^2/day) for steady-state simulation

		ZOOMQ3D	MODFLOW		ZOOMQ3D		MODFLOW		Absolute difference		% difference	
x	y	Groundwater head		Difference	Tx	Ty	Tx	Ty	Tx	Ty	Tx	Ty
0	5000	101.6138	101.614	2.0E-04	2049.972	2049.972	2050.005	2050.005	0.033	0.033	0.002	0.002
500	5000	101.5761	101.576	-1.0E-04	2050.017	2050.017	2050.005	2050.005	0.012	0.012	0.001	0.001
1000	5000	101.4633	101.463	-3.0E-04	2050.057	2050.057	2050.005	2050.005	0.052	0.052	0.003	0.003
1500	5000	102.4304	102.430	-4.0E-04	1950.046	1950.046	1949.985	1949.985	0.061	0.061	0.003	0.003
2000	5000	103.3771	103.377	-1.0E-04	1850.041	1850.041	1850.021	1850.021	0.020	0.020	0.001	0.001
2500	5000	104.3122	104.312	-2.0E-04	1750.019	1750.019	1749.997	1749.997	0.022	0.022	0.001	0.001
3000	5000	105.2487	105.249	3.0E-04	1649.971	1649.971	1650.016	1650.016	0.045	0.045	0.003	0.003
3500	5000	106.2062	106.206	-2.0E-04	1550.015	1550.015	1549.984	1549.984	0.031	0.031	0.002	0.002
4000	5000	107.2142	107.214	-2.0E-04	1450.046	1450.046	1450.026	1450.026	0.020	0.020	0.001	0.001
4500	5000	108.3137	108.314	3.0E-04	1350.347	1350.347	1350.379	1350.379	0.032	0.032	0.002	0.002
5000	5000	110.1211	110.121	-1.0E-04	1250.074	1250.074	1250.068	1250.068	0.006	0.006	0.001	0.001
5500	5000	111.8498	111.850	2.0E-04	1149.967	1149.967	1149.992	1149.992	0.025	0.025	0.002	0.002
6000	5000	113.5149	113.515	1.0E-04	1049.539	1049.539	1049.547	1049.547	0.008	0.008	0.001	0.001
6500	5000	115.1272	115.127	-2.0E-04	949.784	949.784	949.760	949.760	0.024	0.024	0.003	0.003
7000	5000	116.6969	116.697	1.0E-04	849.749	849.749	849.757	849.757	0.008	0.008	0.001	0.001
7500	5000	118.2312	118.231	-2.0E-04	750.094	750.094	750.076	750.076	0.018	0.018	0.002	0.002
8000	5000	119.7337	119.734	3.0E-04	650.228	650.228	650.251	650.251	0.023	0.023	0.004	0.004
8500	5000	121.2052	121.205	-2.0E-04	549.736	549.736	549.723	549.723	0.013	0.013	0.002	0.002
9000	5000	122.6411	122.641	-1.0E-04	450.076	450.076	450.067	450.067	0.009	0.009	0.002	0.002
9500	5000	124.0303	124.030	-3.0E-04	350.013	350.013	349.997	349.997	0.016	0.016	0.005	0.005
10000	5000	125.3485	125.348	-5.0E-04	249.936	249.936	249.914	249.914	0.022	0.022	0.009	0.009
10500	5000	126.5311	126.531	-1.0E-04	150.044	150.044	150.030	150.030	0.014	0.014	0.009	0.009
11000	5000	127.3167	127.317	3.0E-04	49.960	49.978	49.965	49.965	0.005	0.013	0.009	0.026
							Maximum difference		**0.061**	**0.061**	**0.009**	**0.026**

Table 3 Comparison between ZOOMQ3D and MODFLOW river flows for steady-state simulation

River node	River flow (m^3/day) MODFLOW	ZOOMQ3D	Absolute difference (m^3/day)	Difference as % of flow in river
17	0	0	0	0
16	0	0	0	0
15	0	0	0	0
14	0	0	0	0
13	0	0	0	0
12	0	0	0	0
11	0	0	0	0
10	0	0	0	0
9	562.637	562.651	0.014	2.435E-03
8	1699.310	1699.300	0.010	5.885E-04
7	3581.726	3581.720	0.006	1.675E-04
6	6325.149	6325.150	0.001	1.581E-05
5	9686.646	9686.660	0.014	1.445E-04
4	13207.720	13207.800	0.080	6.057E-04
3	16700.680	16700.700	0.020	1.198E-04
2	19533.050	19533.100	0.050	2.560E-04
1	20838.090	20838.100	0.010	4.799E-05

6.3 TEST 2: TIME-VARIANT SIMULATION WITH THE RIVER REMOVED

The second test of ZOOMQ3D is again based on the model shown in Figure 10, however, the river is removed from the model. Consequently, except for the abstraction well which pumps at a constant rate of 8 Ml/day, the only discharge points through which groundwater can leave the system are the leakage nodes. The model simulates a four-year period starting from the beginning of October and uses three time-steps per month of equal length. The storage coefficient is uniform throughout the aquifer and is 0.01. The recharge rates applied during the simulation are listed in Table 4 and shown graphically in Figure 13. The initial groundwater head profile is taken from the MODFLOW test model. This is similar to the steady-state groundwater head profile shown in the previous section. Full details of the model parameters are given in Appendix 1.

Table 4 Recharge rates for Test 2 model (mm/day)

	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep
Year 1	0.627	0.627	0.627	0.627	0.627	0.627	0.627	0.627	0.627	0.627	0.627	0.627
Year 2	0.19355	0.36667	0.16129	1.29030	1.14290	2.32260	1.2	0.19355	0.26667	0.22581	0.06452	0.13333
Year 3	0.19355	0.36667	0.16129	1.29030	1.14290	2.32260	1.2	0.19355	0.26667	0.22581	0.06452	0.13333
Year 4	0.19355	0.36667	0.16129	0.64516	0.78571	1.03230	0.2	0.12903	0.06667	0.06452	0.03226	0.06667

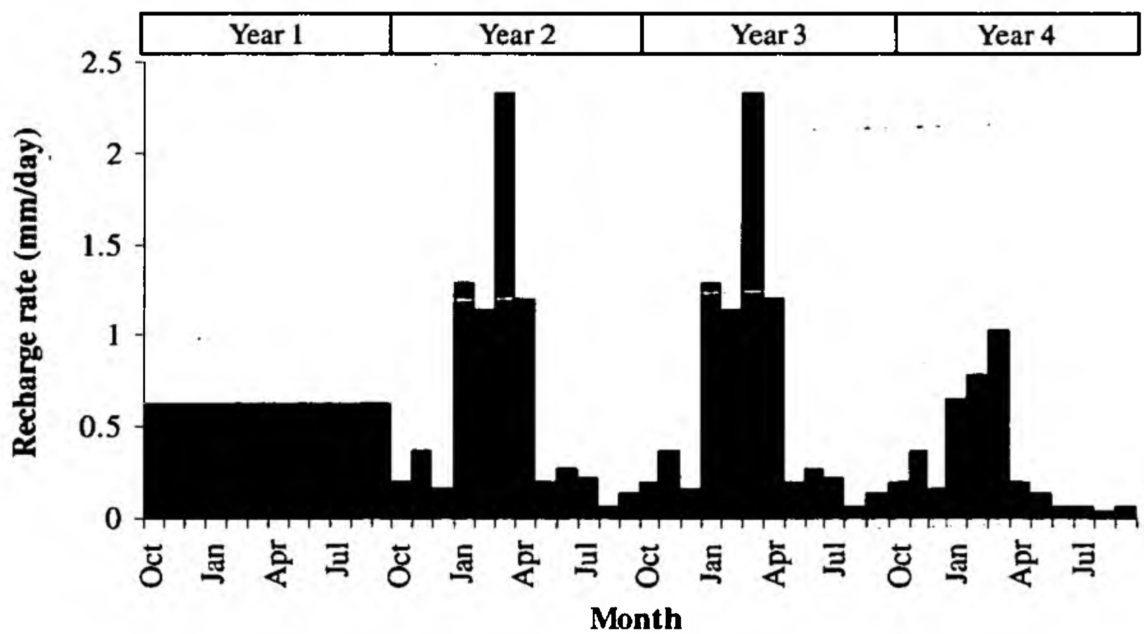


Figure 13 Recharge rates for Test 2 model.

The comparison between the ZOOMQ3D and MODFLOW models is shown graphically in Figures 14 to 17. Figures 14 and 15 show the simulated groundwater hydrographs for the nodes across the centre of the model from left to right. The groundwater hydrographs appear to be in good agreement though it is not possible to infer the exact differences between the two models from these graphs. Figure 16 shows the simulated groundwater head and transmissivity hydrographs at the nodes exhibiting the poorest agreement between the two models. This figure illustrates that acceptance criteria 1 and 2 are met at all of the nodes for all of the 144 time-steps of the simulation. The time-variant global flow balance terms are shown in Figure 17. Only the simulated global flow balance terms are shown. Predefined global flows, such as abstraction and recharge are identical in the two models and therefore are not plotted in the figure. Figure 17d shows that the global flow balance criterion is not violated during the simulation. A summary of the differences between the two models is presented in Table 5. This test indicates that the VKD mechanism has been implemented correctly in ZOOMQ3D. The two models produce very similar results, however, the test model is relatively simple. In the next test, Test 3, an ephemeral river is introduced into the model. This illustrates some subtle but important differences between ZOOMQ3D and MODFLOW.

Table 5 Summary of acceptance criteria values for Test 2 model

Acceptance criterion		Maximum difference	Criterion value	Total number of failures	Average number of failures per time-step
1. Groundwater head (% of head variation)		0.003 % at (10000 m, 5000 m) ≈ 0.001 m	0.5%	0	0
2. Transmissivity	**Tx**	0.054 % at (500 m, 10000 m) ≈ 1.9 m^2/day	1.0%	0	0
	Ty	0.084 % at (11000 m, 2000 m) ≈ 0.017 m^2/day	1.0%	0	0
4. Global flows		0.21 % (storage change)	0.5%	0	0

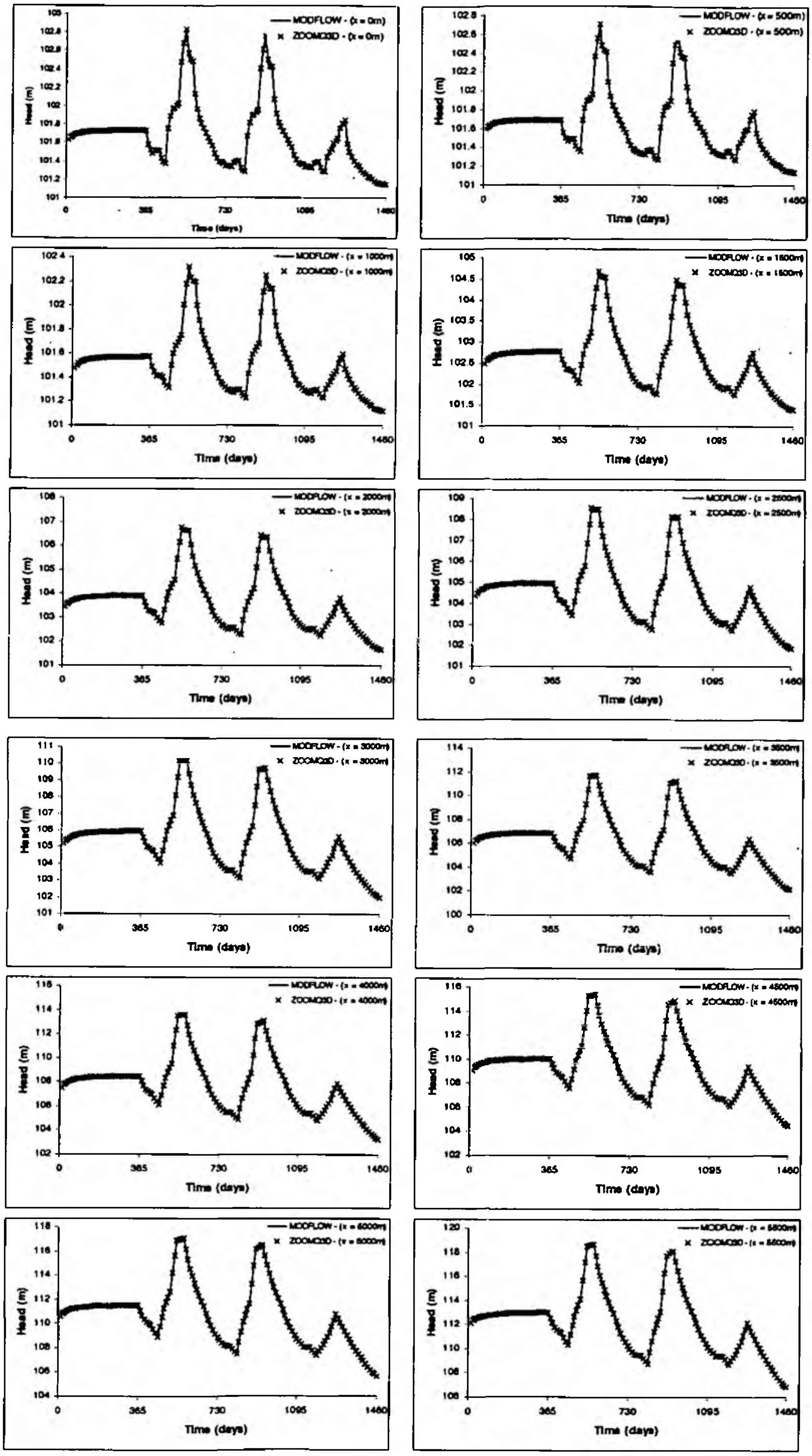


Figure 14 Simulated groundwater heads across the centre of the grid (y=5000 m) for the Test 2 model

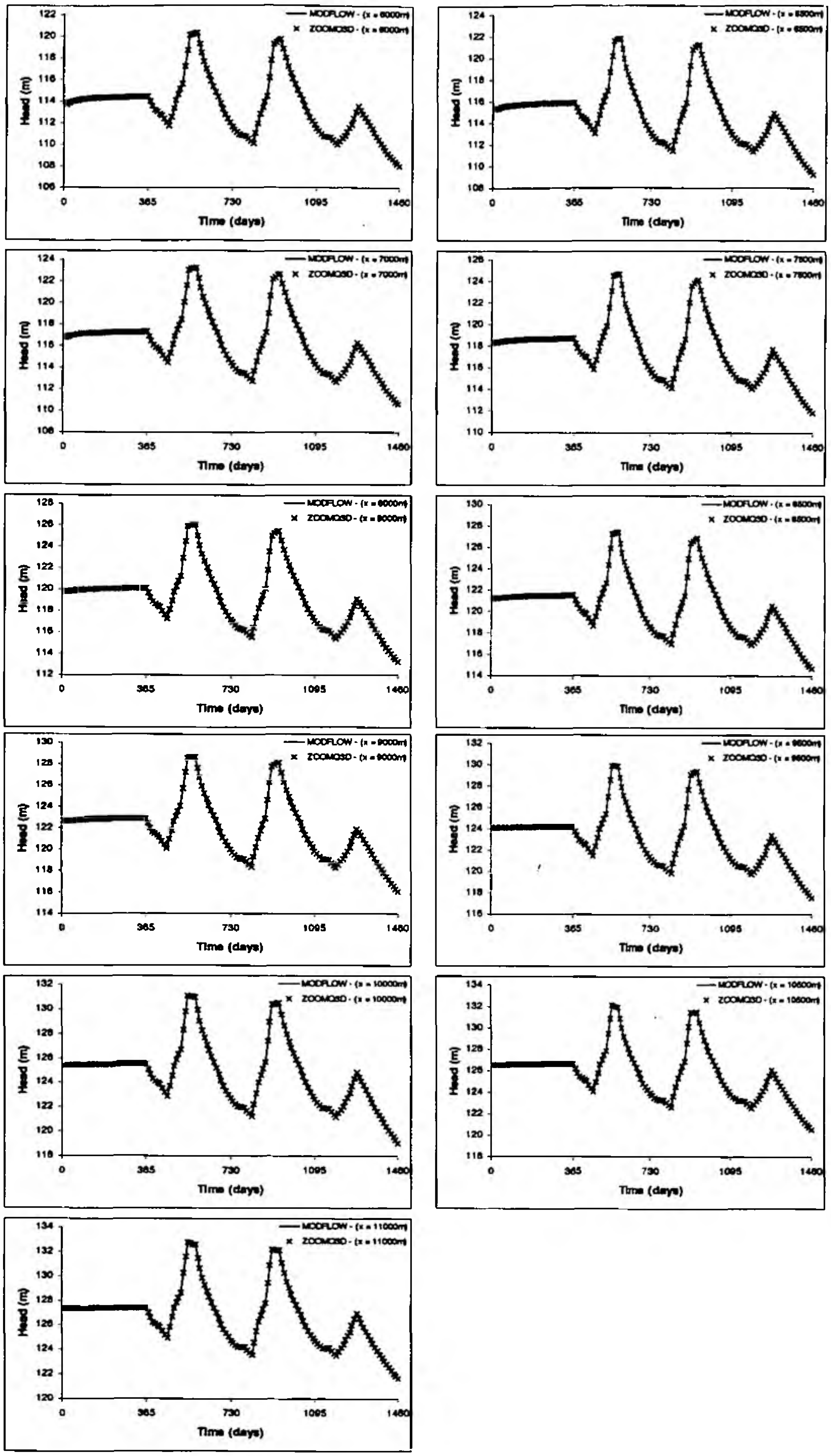


Figure 15 Simulated groundwater heads across the centre of the grid (y=5000 m) for the Test 2 model

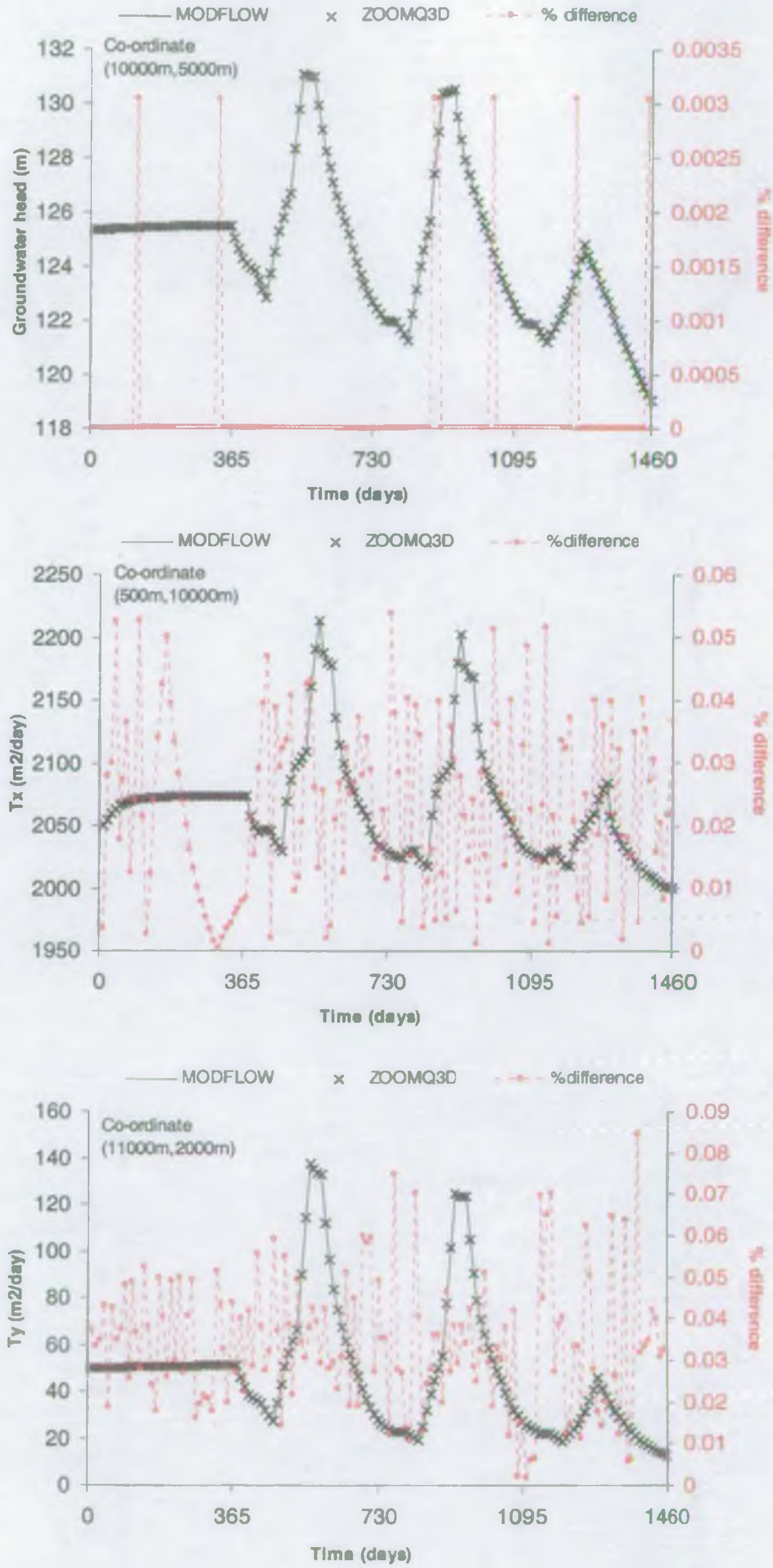
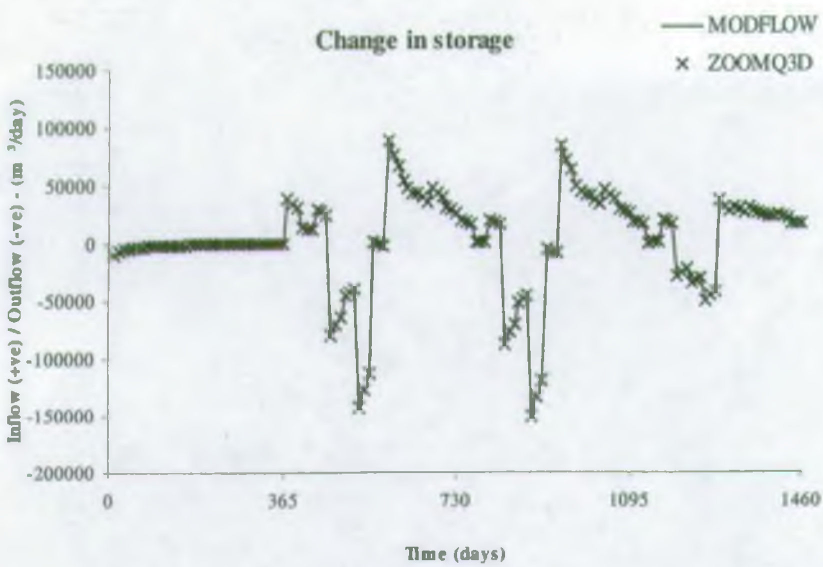
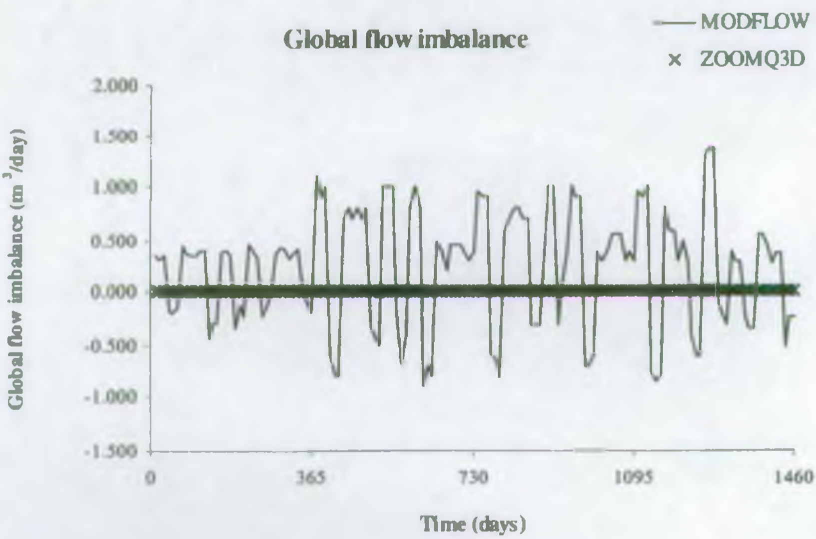


Figure 16 Simulated groundwater head and transmissivity hydrographs at the nodes of the Test 2 model that exhibit the greatest differences between ZOOMQ3D and MODFLOW

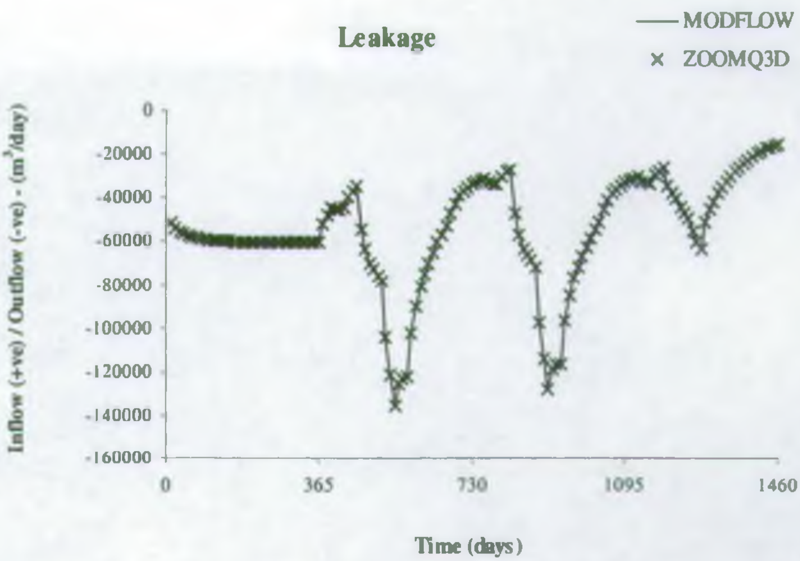


a)



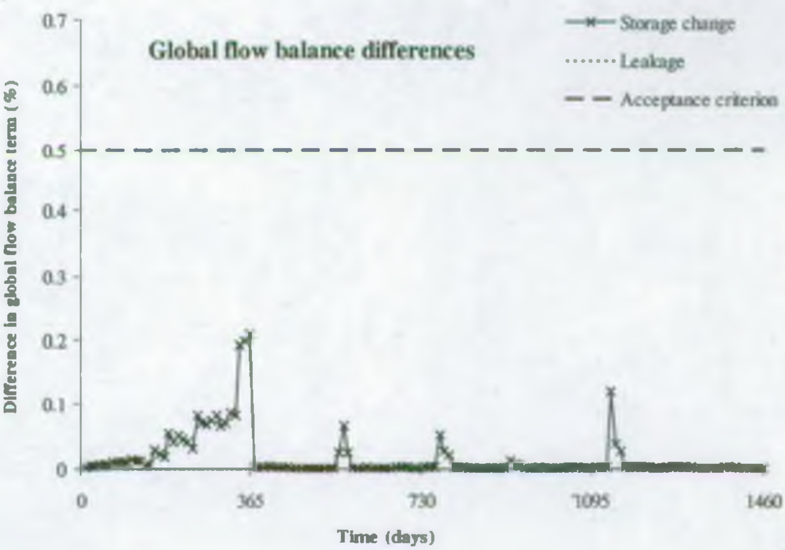
c)

Figure 17 Simulated global flows for each feature of the Test 2 model



Leakage
MODFLOW
ZOOMQ3D
Inflow (+ve) / Outflow (-ve) - (m3/day)
0
-20000
-40000
-60000
-80000
-100000
-120000
-140000
-160000
0
365
730
1095
1460
Time (days)

b)



Global flow balance differences
Storage change
Leakage
Acceptance criterion
Difference in global flow balance term (%)
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
365
730
1095
1460
Time (days)

d)

6.4 TEST 3: TIME-VARIANT SIMULATION MODEL INCORPORATING THE EPHEMERAL RIVER

In this test, the river, which runs approximately between the bottom right and the top left corners of the grid, is reintroduced into the model. This is shown in Figure 10. A constant discharge of 2700 m^3/day flows into the river at co-ordinate (9500 m, 3500 m). Both ZOOMQ3D and MODFLOW simulate the accreted flow in the river. All other model parameters are the same as in the Test 2 model. Again, a four-year period is simulated using the recharge pattern shown in Figure 13. Three simulations are performed using the Test 3 model: Test 3a to 3c. The simulations illustrate the subtle but important differences by which ZOOMQ3D and MODFLOW simulate unconfined conditions and ephemeral rivers.

6.4.1 Test 3a

In this simulation, the first using the Test 3 model, an *explicit* representation of the variation of transmissivity in time is used by both ZOOMQ3D and MODFLOW. That is, the transmissivity for the current time-step is calculated using the groundwater head at the end of the last time-step. At the end of the current time-step transmissivity is recalculated. This is a commonly applied method for simulating unconfined aquifers.

The comparison between the two models is shown in Figures 18 to 22. In Figures 18 and 19 the groundwater head hydrographs are plotted for the seventeen nodes along the river. In Figures 20 and 21 the river flow hydrographs are shown for the seventeen nodes. The groundwater hydrographs simulated by ZOOMQ3D for the nodes along the river show varying degrees of agreement with those simulated by MODFLOW. An initial inspection of the groundwater hydrographs for the rivers nodes downstream of river node 11, which are shown in Figure 18, appears to indicate that there is satisfactory agreement between the two models. However, the groundwater hydrographs for river nodes 11 to 17 at the upstream end of the river show significant differences between the two models. Such significant differences are not observed in the river flow hydrographs, though it is difficult to infer the exact level of agreement between the two models from these plots. An indication of the cause of the differences between the two models is given by specific anomalies that can be identified on the groundwater hydrographs. These are highlighted by dashed circles in Figures 18 and 19. These anomalies occur on the rising limbs of the groundwater hydrographs. The dashed circles on Figures 18 and 19 show that the groundwater head rises more sharply in the ZOOMQ3D model than the MODFLOW model at particular time-steps. This behaviour is related to the way in which ZOOMQ3D and MODFLOW simulate ephemeral rivers.

In both ZOOMQ3D and MODFLOW a dry river node begins to flow again when the groundwater head at that point rises above the river bed. However, the frequency with which this is checked for differs between the two models. MODFLOW allows the coefficients of the finite difference equations to be modified whilst the solution of the set of simultaneous equations is calculated. That is, leakage from the aquifer to the river can be switched back on between *iterations* of a numerical solution algorithm, for example, successive over-relaxation. A second example of such a modification is that of transmissivity, which can also be updated between iterations when simulating unconfined aquifers. The modification of the coefficients between iterations can be problematic because whilst the equations are being solved they are being changed. For many problems this method is acceptable, however, on occasions the technique does not converge. ZOOMQ3D is stricter because the finite difference equations cannot be modified during the solution procedure. Consequently, dry river nodes can only be allowed to re-wet at the end of a time-step or time-step cycle. That is, the terms relating to the head dependent leakage of water from the aquifer to a dry river node can only be added to the finite difference equation for that grid node at the end of a time-step. This rule causes the jumps that are observed in the groundwater hydrographs simulated by ZOOMQ3D shown in Figure 18 and

Figure 19. The difference between the two models is illustrated by examining Table 6, which lists the flow and groundwater head along the river simulated by both ZOOMQ3D and MODFLOW at the end of three time-steps.

Table 6 Simulated river flows and groundwater heads by ZOOMQ3D and MODFLOW Test 3a models

	Time (days)	457	467.333	477.667	457	467.333	477.667
		ZOOMQ3D river flow (m^3/day)			MODFLOW river flow (m^3/day)		
	17	0	0	0	0	0	0
	16	0	0	0	0	0	0
Upstream	15	1500	1500	1500	1500	1500	1500
	14	0	0	0	0	0	0
	13	0	0	0	0	0	0
	12	0	0	0	0	0	0
	11	0	0	0	0	0	0
River node	10	0	0	0	0	0	0
	9	0	0	0	0	0	31.40
	8	0	0	0	0	0	469.80
	7	0	0	0	0	0	1385.93
	6	0	0	2116.56	0	848.33	3200.64
	5	651.60	2230.76	5084.69	651.58	2924.10	6066.47
	4	2131.03	5034.40	8583.07	2130.98	5689.32	9524.55
Downstream	3	3988.60	8112.75	12277.60	3988.54	8755.19	13201.90
	2	5511.72	10745.20	15429.00	5511.66	11383.20	16346.00
	1	5817.92	12007.60	17096.00	5817.81	12644.20	18010.00

		Time (days)	457	467.333	477.667	457	467.333	477.667
		River bed Elevation	ZOOMQ3D groundwater head (m)			MODFLOW groundwater head (m)		
	17	130	122.25	123.14	123.98	122.25	123.14	123.979
	16	127.6	121.184	122.081	122.912	121.184	122.081	122.911
Upstream	15	125.2	120.713	121.643	122.395	120.713	121.642	122.392
	14	122.8	119.26	120.187	120.942	119.26	120.187	120.936
	13	120.4	117.067	117.969	118.789	117.067	117.967	118.778
	12	118	115.239	116.129	116.961	115.239	116.126	116.943
	11	116	113.566	114.451	115.276	113.566	114.446	115.243
River node	10	114	111.976	112.857	113.664	111.976	112.849	113.609
	9	112	110.443	111.318	112.099	110.442	111.306	112.005
	8	110	108.756	109.612	110.315	108.756	109.583	110.073
	7	108	107.15	107.955	108.483	107.15	107.884	108.153
	6	106.1	105.804	106.486	106.453	105.804	106.241	106.402
	5	104.5	104.609	104.872	104.995	104.609	104.846	104.978
	4	103.3	103.547	103.767	103.883	103.547	103.761	103.876
Downstream	3	102.4	102.71	102.913	103.016	102.71	102.911	103.013
	2	101.9	102.154	102.339	102.425	102.154	102.338	102.424
	1	101.75	101.801	101.96	102.028	101.801	101.96	102.027

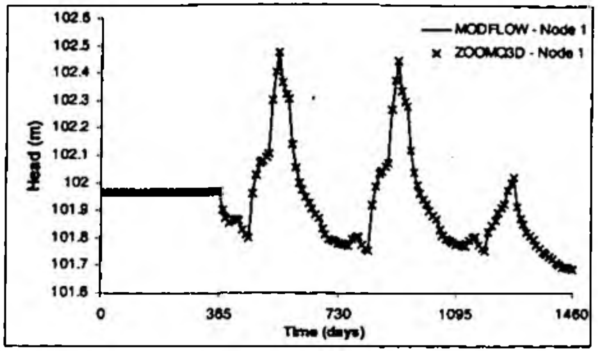
Table 6 shows that at the end of first time-step listed, after 457 days of the simulation, there are only minor differences between the river flows simulated by ZOOMQ3D and MODFLOW. However, during the second time-step listed, between 457 and 467.333 days, river node 6 begins to flow in the MODFLOW model but not in the ZOOMQ3D model. In both models the groundwater head rises above the river bed at this point, however, leakage to the river is only 'switched back on' in the MODFLOW model. The consequence of this is that groundwater head rises more significantly at river node 6 in the ZOOMQ3D model because water cannot leave the aquifer at this point. River node 6 is reconnected to the aquifer at the end of the time-step in the ZOOMQ3D model after which time the river node begins to flow again. The same phenomenon occurs between the second and third time-steps listed when more MODFLOW river nodes re-wet but ZOOMQ3D river nodes do not.

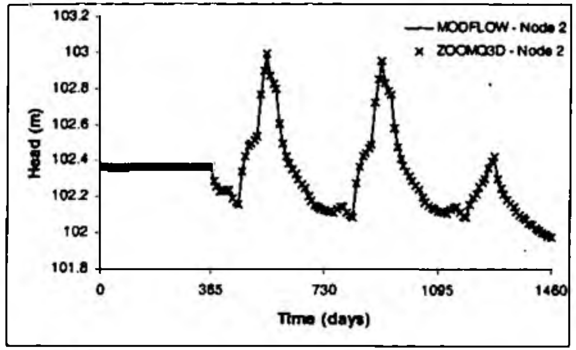
Figure 22 shows the groundwater head and transmissivity hydrographs at the nodes that show the poorest agreement between the two models. In terms of groundwater head this occurs at the node located at the upstream end of the river. Acceptance criteria 1 and 2 relating to the variation in groundwater head and transmissivity are substantially violated during the simulation at these nodes. The degree to which the model violates the acceptance criteria is summarised in Table 7.

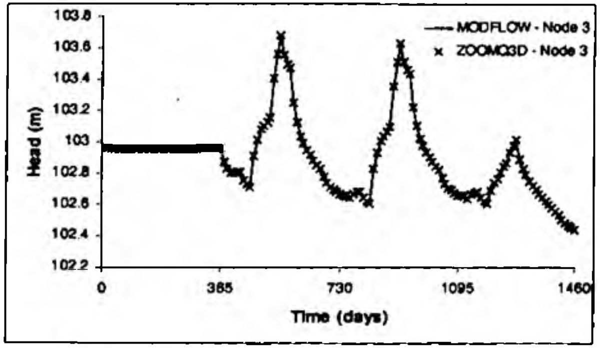
Table 7 Summary of acceptance criteria values for Test 3a model

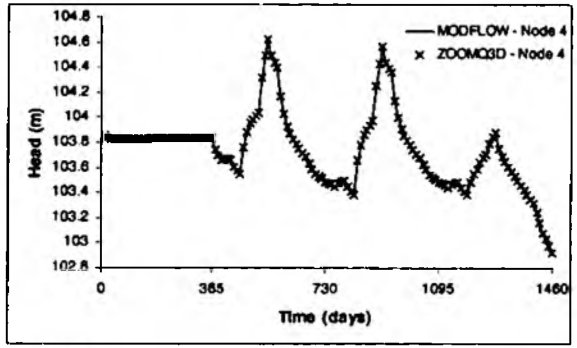
Acceptance criterion		Maximum difference	Criterion value	Total number of failures	Average number of failures per time-step
1. Groundwater head		6.3 % at (9500 m, 2500 m)	0.5%	10649	74.0
(% of head variation)		≈ 2.1 m			
2. Transmissivity	Tx	10.1 % at (7500 m, 4000 m)	1.0%	117	0.81
		≈ 97.5 m^2/day			
	Ty	9.1 % at (8000 m, 4000 m)	1.0%	118	0.82
		≈ 86.8 m^2/day			
3. River flow		11.2 %	2.0%	65	0.45
(% of max accreted flow)		≈ 892 m^3/day			

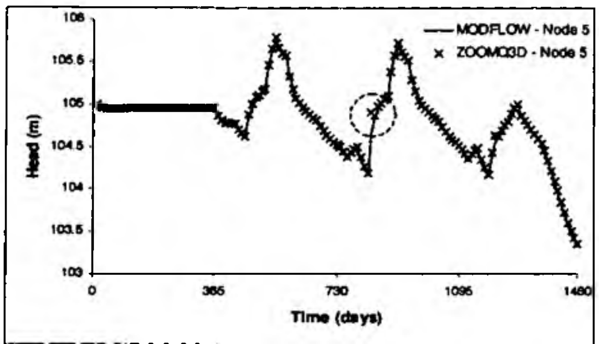
Whilst, significant discrepancies are observed between the ZOOMQ3D and MODFLOW models in this test, the cause of these is well understood. They are due to the models using different techniques to update the finite difference equations when dry river nodes re-wet. This results in these river nodes re-wetting at different times. A limitation of ZOOMQ3D is that dry river nodes can only be 'reconnected' to the aquifer at the end of the solution of a time-step. However, this approach has been adopted in preference to the modification of the finite difference equations between the *iterations* of a solution algorithm. The problem of river nodes not re-wetting at the correct time-step can be solved by using multiple time-step *cycles* within ZOOMQ3D as described in Section 6.4.3. The comparison of the MODFLOW model with a ZOOMQ3D model which uses multiple time-step cycles and transmissivity updating is the subject of the next section.

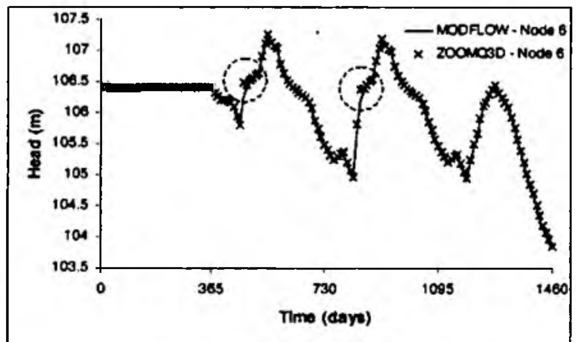

MODFLOW - Node 1
ZOOMQ3D - Node 1
Head (m)
Time (days)


MODFLOW - Node 2
ZOOMQ3D - Node 2
Head (m)
Time (days)


MODFLOW - Node 3
ZOOMQ3D - Node 3
Head (m)
Time (days)


MODFLOW - Node 4
ZOOMQ3D - Node 4
Head (m)
Time (days)


MODFLOW - Node 5
ZOOMQ3D - Node 5
Head (m)
Time (days)


MODFLOW - Node 6
ZOOMQ3D - Node 6
Head (m)
Time (days)

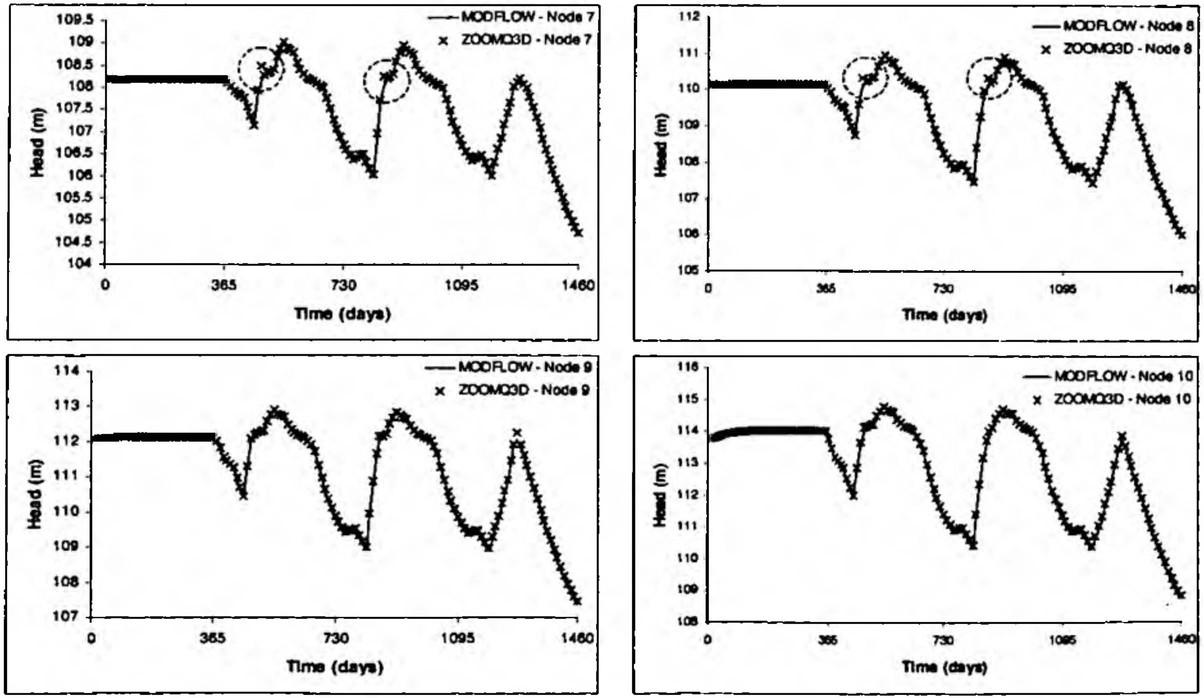
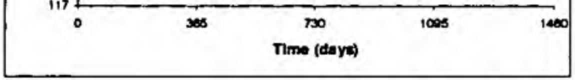
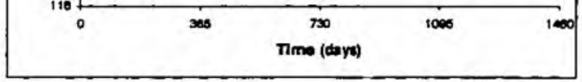


Figure 18 Simulated groundwater heads long river channel in Test 3a

(Node 1 at the downstream end of the river)





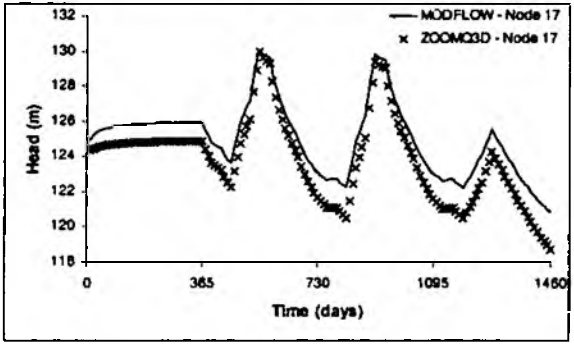
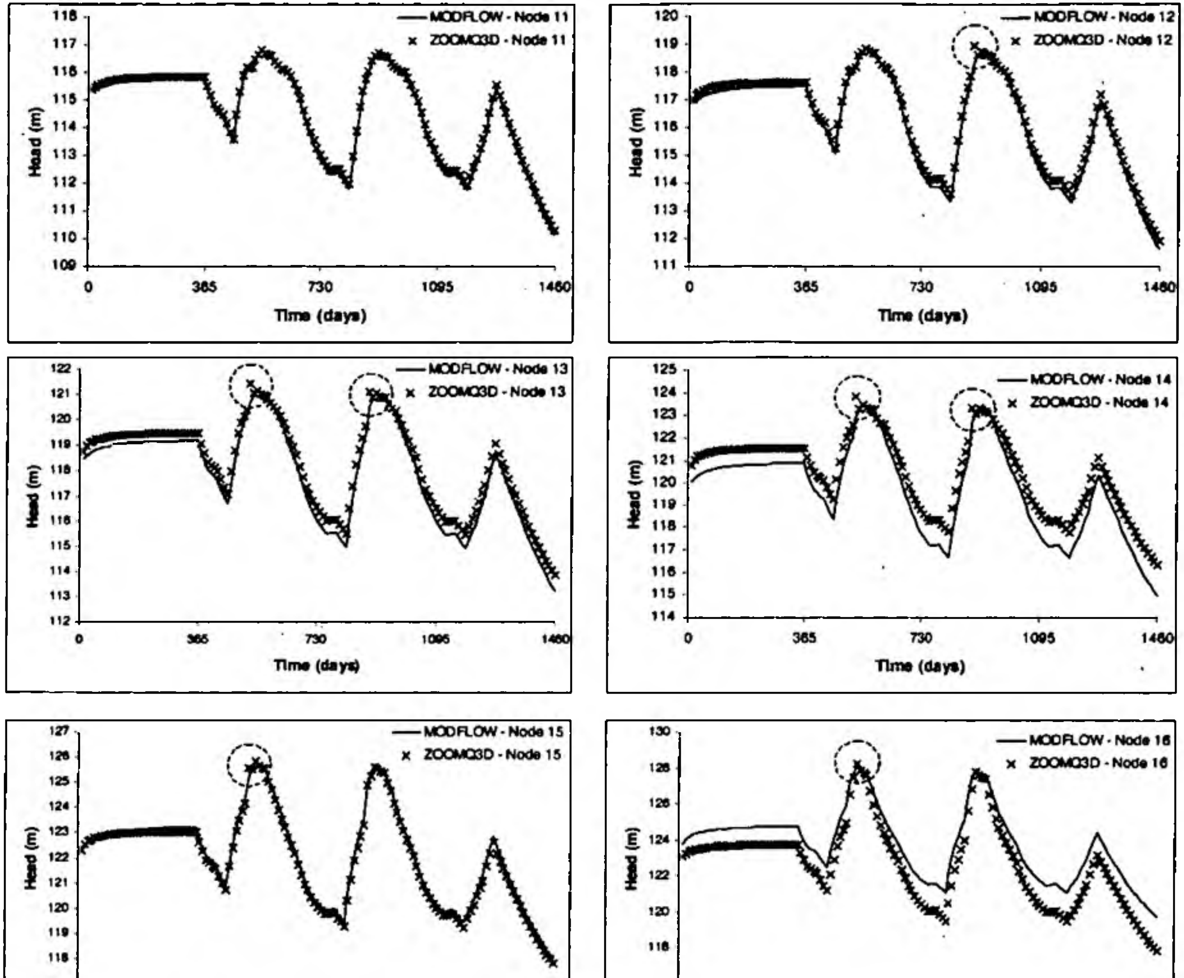


Figure 19 Simulated groundwater heads long river channel in Test 3a

(Node 17 at the upstream end of the river)



MODFLOW - Node 11
ZOOMQ3D - Node 11
MODFLOW - Node 12
ZOOMQ3D - Node 12
MODFLOW - Node 13
ZOOMQ3D - Node 13
MODFLOW - Node 14
ZOOMQ3D - Node 14
MODFLOW - Node 15
ZOOMQ3D - Node 15
MODFLOW - Node 16
ZOOMQ3D - Node 16
Head (m)
Time (days)
0
365
730
1095
1460

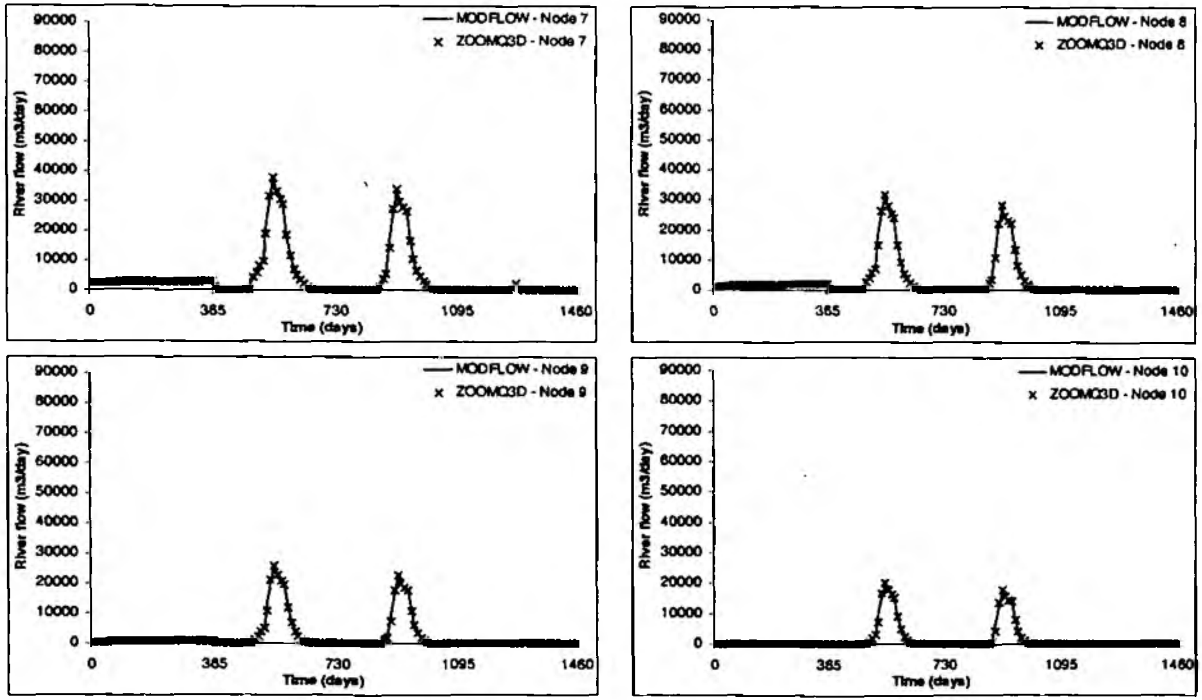
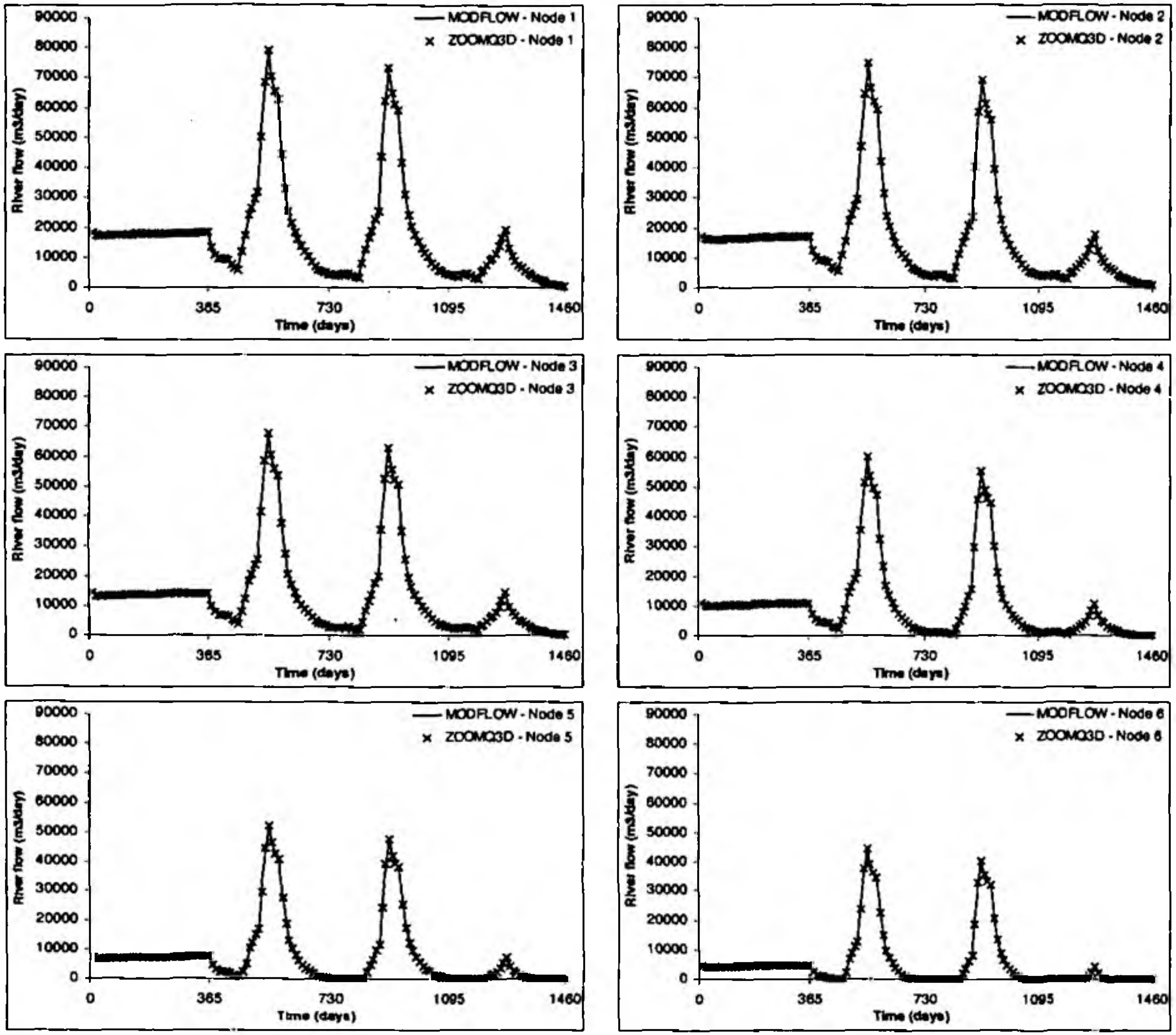


Figure 20 Simulated river flows in Test 3a

(Node 1 at the downstream end of the river)



MODFLOW - Node 1
ZOOMQ3D - Node 1
MODFLOW - Node 2
ZOOMQ3D - Node 2
MODFLOW - Node 3
ZOOMQ3D - Node 3
MODFLOW - Node 4
ZOOMQ3D - Node 4
MODFLOW - Node 5
ZOOMQ3D - Node 5
MODFLOW - Node 6
ZOOMQ3D - Node 6
River flow (m3/day)
Time (days)
0
10000
20000
30000
40000
50000
60000
70000
80000
90000
0
365
730
1095
1460

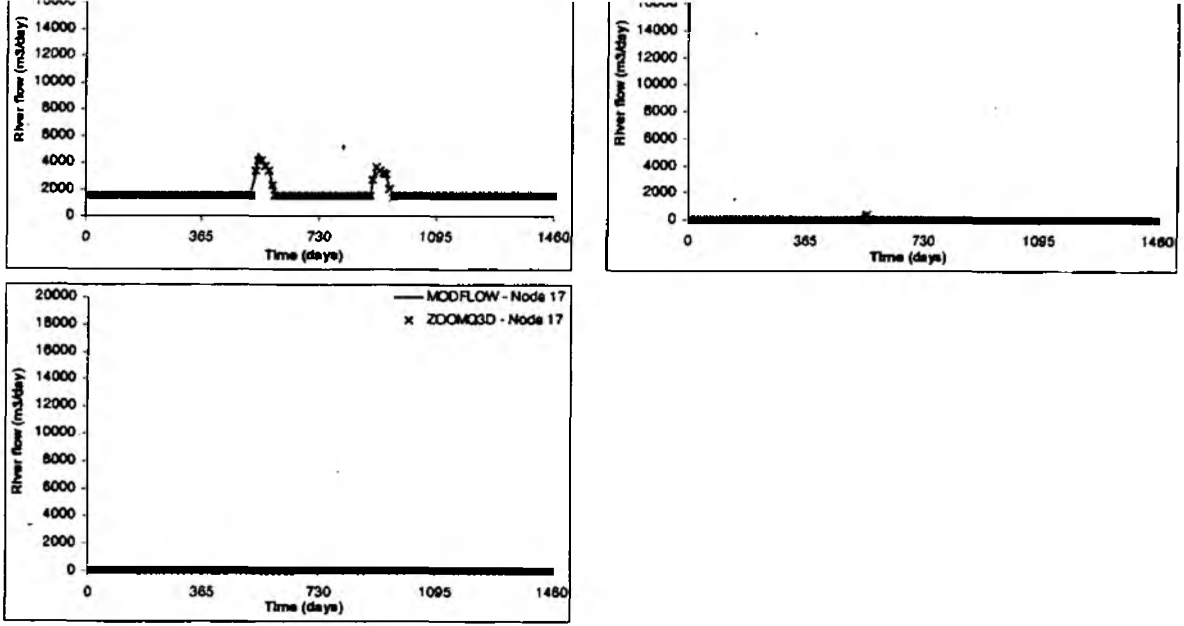
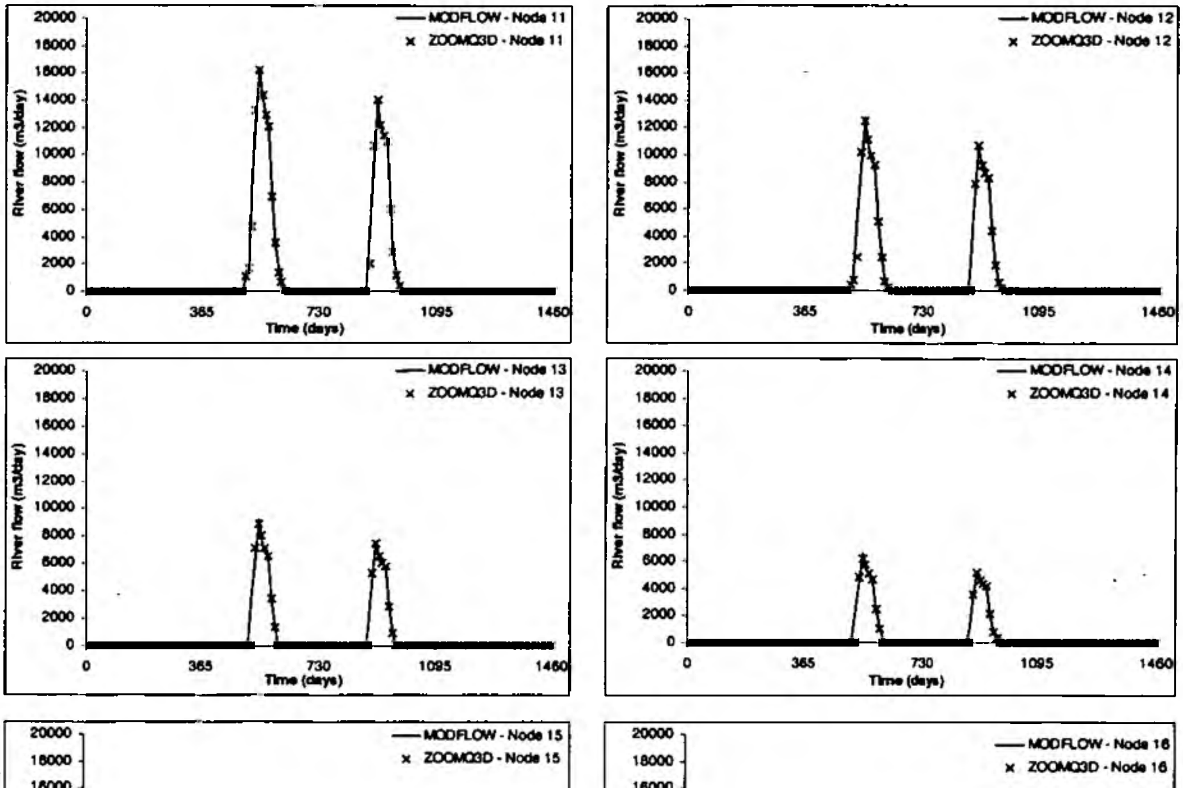


Figure 21 Simulated river flows in Test 3a

(Node 17 at the upstream end of the river)


River flow (m3/day)
Time (days)
MODFLOW - Node 11
ZOOMQ3D - Node 11
MODFLOW - Node 12
ZOOMQ3D - Node 12
MODFLOW - Node 13
ZOOMQ3D - Node 13
MODFLOW - Node 14
ZOOMQ3D - Node 14
MODFLOW - Node 15
ZOOMQ3D - Node 15
MODFLOW - Node 16
ZOOMQ3D - Node 16

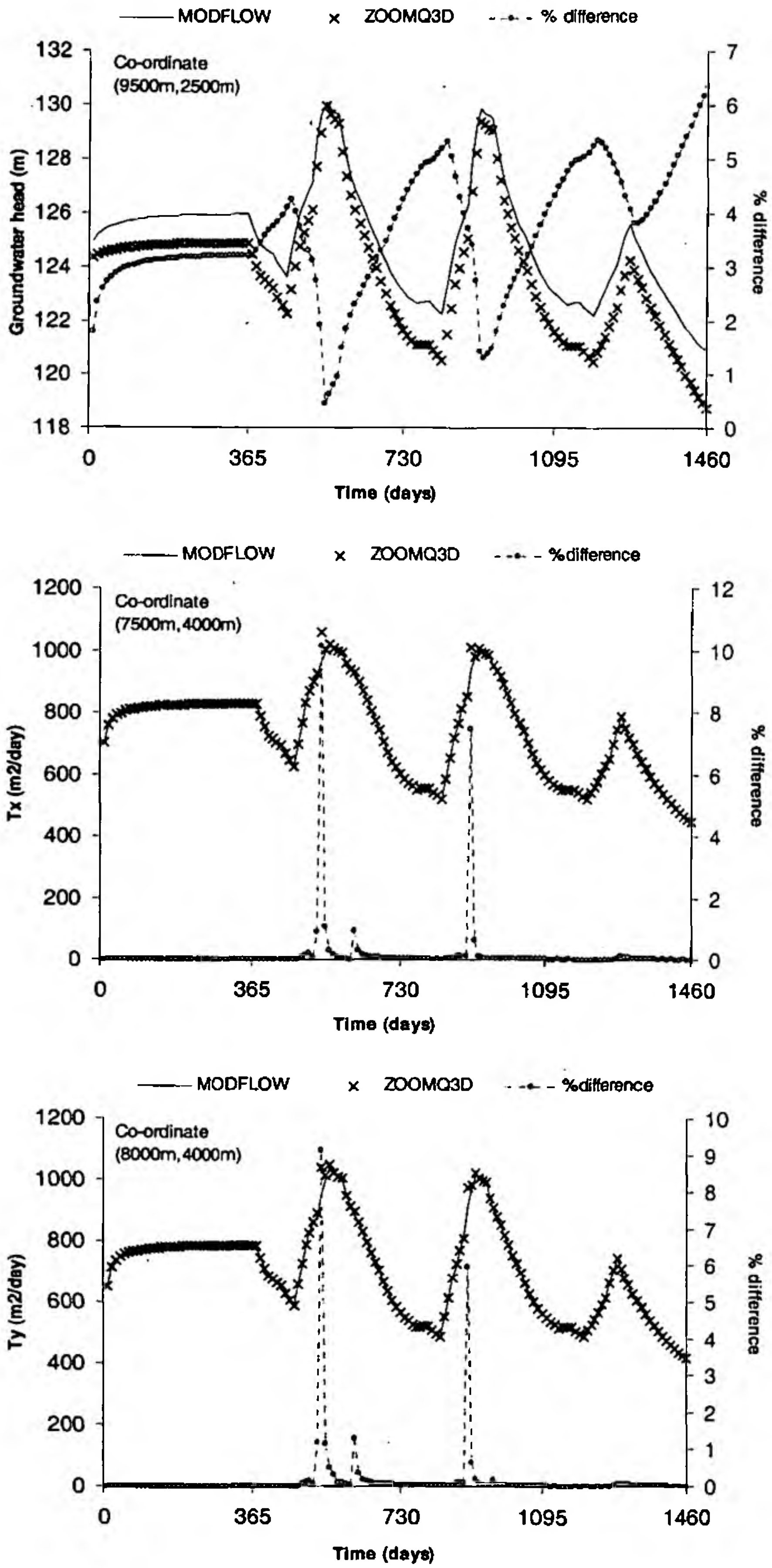


Figure 22 Simulated groundwater head and transmissivity hydrographs at the nodes of the Test 3a model that exhibit the greatest differences between ZOOMQ3D and MODFLOW

6.4.2 Test 3b

The MODFLOW model used in this test is identical to the one described in the previous section. The ZOOMQ3D model is identical except for one change. In the previous ZOOMQ3D model the solution at a time-step is calculated only once. Transmissivity for the current time-step is based on the groundwater head at the end of the last time-step, just as in the MODFLOW model. However, in the ZOOMQ3D Test 3b model, multiple time-step cycles are used. This is explained in Section 5. The model calculates the solution for a single time-step a number of times. At the end of a cycle, transmissivity is updated. The transmissivity at a node is calculated as the average of that based on the current head and that based on the head at the end of the last cycle. At the end of a time-step *cycle* the terms contained in the finite difference equations that relate to river-aquifer interaction can be updated. Using this method, dry river nodes can re-wet *during* a time-step when the groundwater head rises above the river bed. This is not possible when a single time-step cycle is used as in the previous test, Test 3a. Consequently, in this test both models allow dry river nodes to re-wet during a time-step. However, transmissivity is updated differently in the two models. In MODFLOW transmissivity is updated at the beginning of a time-step whereas in ZOOMQ3D transmissivity is updated at the beginning of a cycle and there are multiple cycles per time-step.

The comparison between the ZOOMQ3D and MODFLOW models is shown in Figures 23 to 27. In Figures 23 and 24 the groundwater head hydrographs are plotted for the seventeen nodes along the river. In Figures 25 and 26 the flow hydrographs are shown for the seventeen river nodes. The groundwater hydrographs simulated by ZOOMQ3D for the nodes along the river again show varying degrees of agreement with those simulated by MODFLOW. The groundwater hydrographs for the rivers nodes downstream of river node 11, which are shown in Figure 23, appear to indicate that there is satisfactory agreement between the two models. However, the groundwater hydrographs for river nodes 11 to 17 at the upstream end of the river again show significant differences between the two models. The river flow hydrographs do not appear to show such significant differences. The sharp rises in groundwater head that are simulated by the previous Test 3a model on the rising limb of the hydrographs, are not produced by this ZOOMQ3D model. This is because dry river nodes can re-wet during a time-step. To illustrate this, Table 8 shows the simulated river flows at the same times as those listed in Table 6, which relates to the previous test. Table 8 shows that each of the nodes of the ZOOMQ3D and MODFLOW models re-wet at the same time during the three time-steps listed.

In this test the differences between the ZOOMQ3D and MODFLOW models are not due to the representation of ephemeral rivers. Instead they are due to differences in the calculation of transmissivity during the simulation. In MODFLOW, transmissivity at a node is calculated at the beginning of a time-step and is constant during the calculation of the solution for the time-step. That is, transmissivity is not updated between *iterations* of the numerical solution algorithm. However, in ZOOMQ3D transmissivity is updated at the end of each cycle of which there are a number per time-step.

Figure 27 shows the groundwater head and transmissivity hydrographs at the nodes of the model that show the poorest agreement between the two models. In terms of groundwater head this again occurs at the node located at the upstream end of the river. Acceptance criteria 1 and 2 relating to the variation in groundwater head and transmissivity are often violated during the simulation at these nodes. The degree to which the model violates the acceptance criteria is summarised in Table 9.

Table 8 Simulated river flows and groundwater heads by ZOOMQ3D and MODFLOW Test 3b models

	Time (days)	457	467.333	477.667	457	467.333	477.667
		ZOOMQ3D river flow (m^3/day)			MODFLOW river flow (m^3/day)		
	17	0	0	0	0	0	0
	16	0	0	0	0	0	0
Upstream	15	1500	1500	1500	1500	1500	1500
	14	0	0	0	0	0	0
	13	0	0	0	0	0	0
	12	0	0	0	0	0	0
	11	0	0	0	0	0	0
River node	10	0	0	0	0	0	0
	9	0	0	77.9076	0	0	31.4026
	8	0	0	603.17	0	0	469.803
	7	0	0	1633.8	0	0	1385.93
	6	0	941.956	3570.11	0	848.328	3200.64
	5	604.448	3103.42	6550.97	651.581	2924.1	6066.47
	4	2049.45	5947.96	10112.2	2130.98	5689.32	9524.55
Downstream	3	3879.52	9089.92	13880.5	3988.54	8755.19	13201.9
	2	5381.49	11782.1	17098.2	5511.66	11383.2	16346
	1	5672.93	13088.2	18814.2	5817.81	12644.2	18010

		Time (days)	457	467.333	477.667	457	467.333	477.667
		River bed Elevation	ZOOMQ3D groundwater head (m)			MODFLOW groundwater head (m)		
	17	130	122.371	123.204	123.982	123.605	124.543	125.316
	16	127.6	121.3	122.127	122.894	122.454	123.394	124.154
Upstream	15	125.2	120.838	121.601	122.295	120.879	121.81	122.573
	14	122.8	119.375	120.14	120.838	118.347	119.239	120.075
	13	120.4	117.156	117.981	118.737	116.663	117.547	118.382
	12	118	115.305	116.154	116.932	115.032	115.91	116.735
	11	116	113.613	114.472	115.248	113.45	114.324	115.126
River node	10	114	112.006	112.87	113.62	111.908	112.777	113.544
	9	112	110.456	111.324	112.013	110.402	111.262	111.979
	8	110	108.753	109.604	110.088	108.721	109.546	110.062
	7	108	107.134	107.912	108.172	107.122	107.859	108.145
	6	106.1	105.784	106.257	106.423	105.786	106.234	106.397
	5	104.5	104.601	104.86	104.997	104.604	104.842	104.974
	4	103.3	103.541	103.774	103.894	103.544	103.758	103.874
Downstream	3	102.4	102.705	102.924	103.028	102.708	102.909	103.011
	2	101.9	102.15	102.349	102.436	102.153	102.337	102.423
	1	101.75	101.799	101.968	102.036	101.8	101.959	102.026

As with the previous test model, whilst significant discrepancies are observed between the ZOOMQ3D and MODFLOW models the cause of these is well understood. In this test they are due to difference in the updating of transmissivity during the simulation. In the next section the final test using the model shown in Figure 10 is described. The comparison is made between the MODFLOW model and the ZOOMQ3D model, which update transmissivity in the same way and which both allow dry river nodes to re-wet immediately after the groundwater head rises above the river bed.

Table 9 Summary of acceptance criteria values for Test 3b model

Acceptance criterion		Maximum difference	Criterion value	Total number of failures	Average number of failures per time-step
1. Groundwater head		5.9 % at (9500 m, 2500 m)	0.5%	14128	98.1
(% of head variation)		≈ 2.0 m			
2. Transmissivity	**Tx**	31.4 % at (7500 m, 4000 m)	1.0%	33404	232.0
		≈ 33.3 m^2/day			
	Ty	34.0 % at (8000 m, 4000 m)	1.0%	32832	228.0
		≈ 6.4 m^2/day			
3. River flow		5.8 %	2.0%	280	1.9
(% of max accreted flow)		≈ 2415.8 m^3/day			

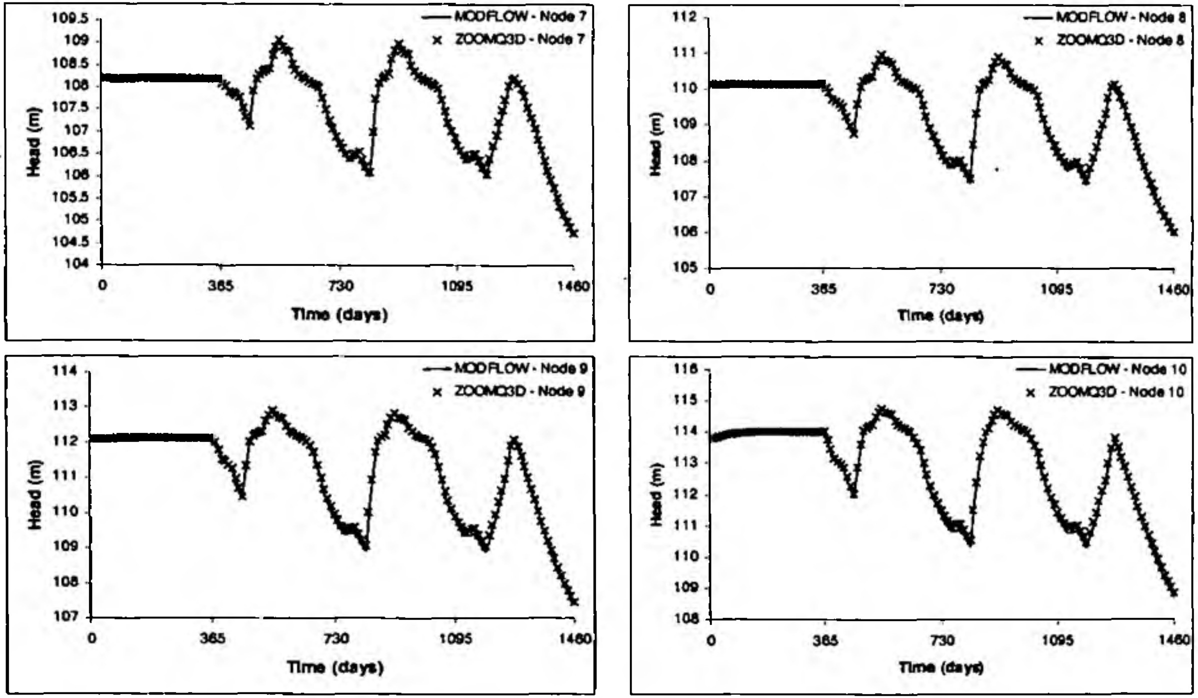
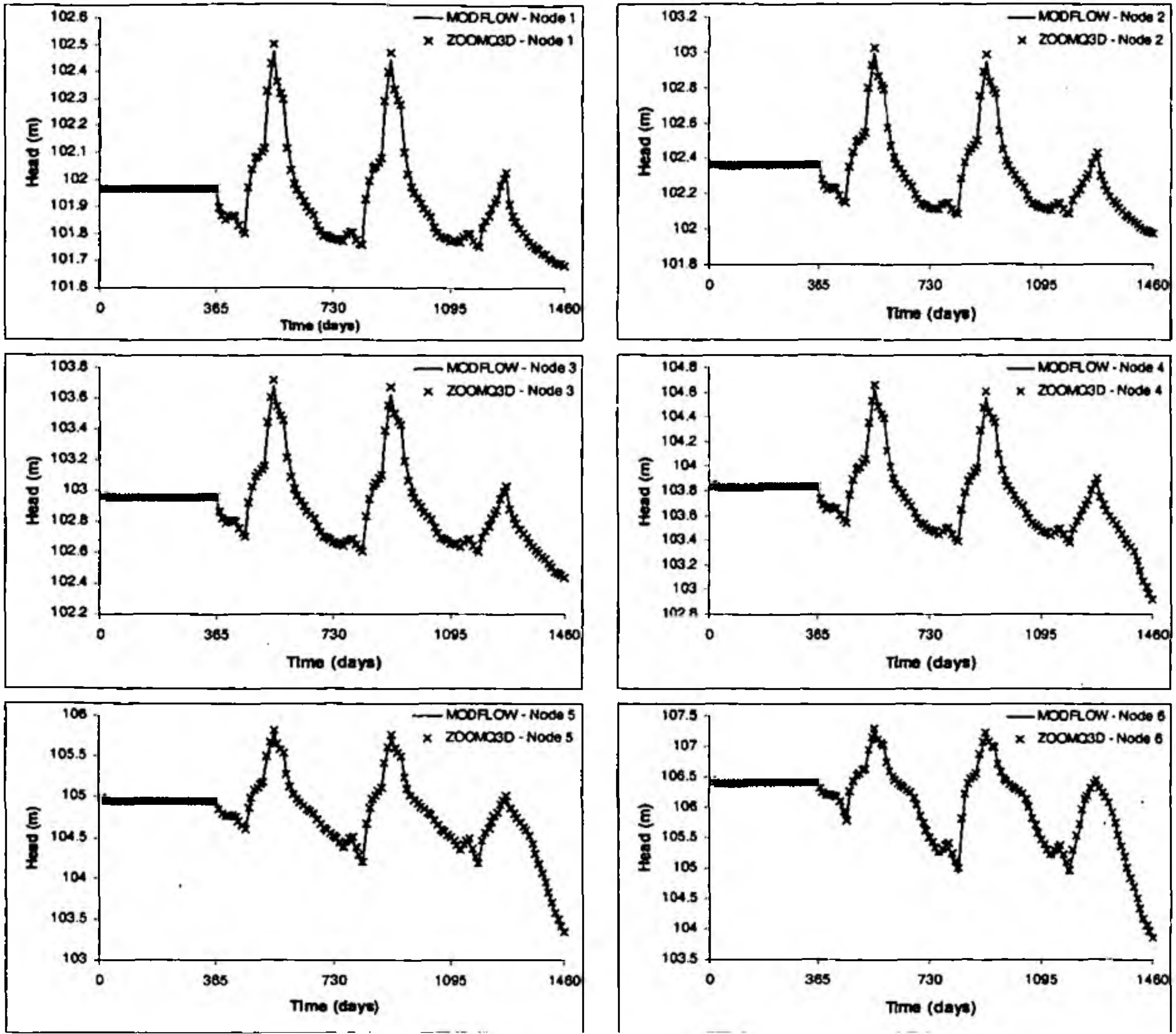


Figure 23 Simulated groundwater heads long river channel in Test 3b

(Node 1 at the downstream end of the river)


MODFLOW - Node 1
ZOOMQ3D - Node 1
MODFLOW - Node 2
ZOOMQ3D - Node 2
MODFLOW - Node 3
ZOOMQ3D - Node 3
MODFLOW - Node 4
ZOOMQ3D - Node 4
MODFLOW - Node 5
ZOOMQ3D - Node 5
MODFLOW - Node 6
ZOOMQ3D - Node 6
Head (m)
Time (days)
0
365
730
1095
1460

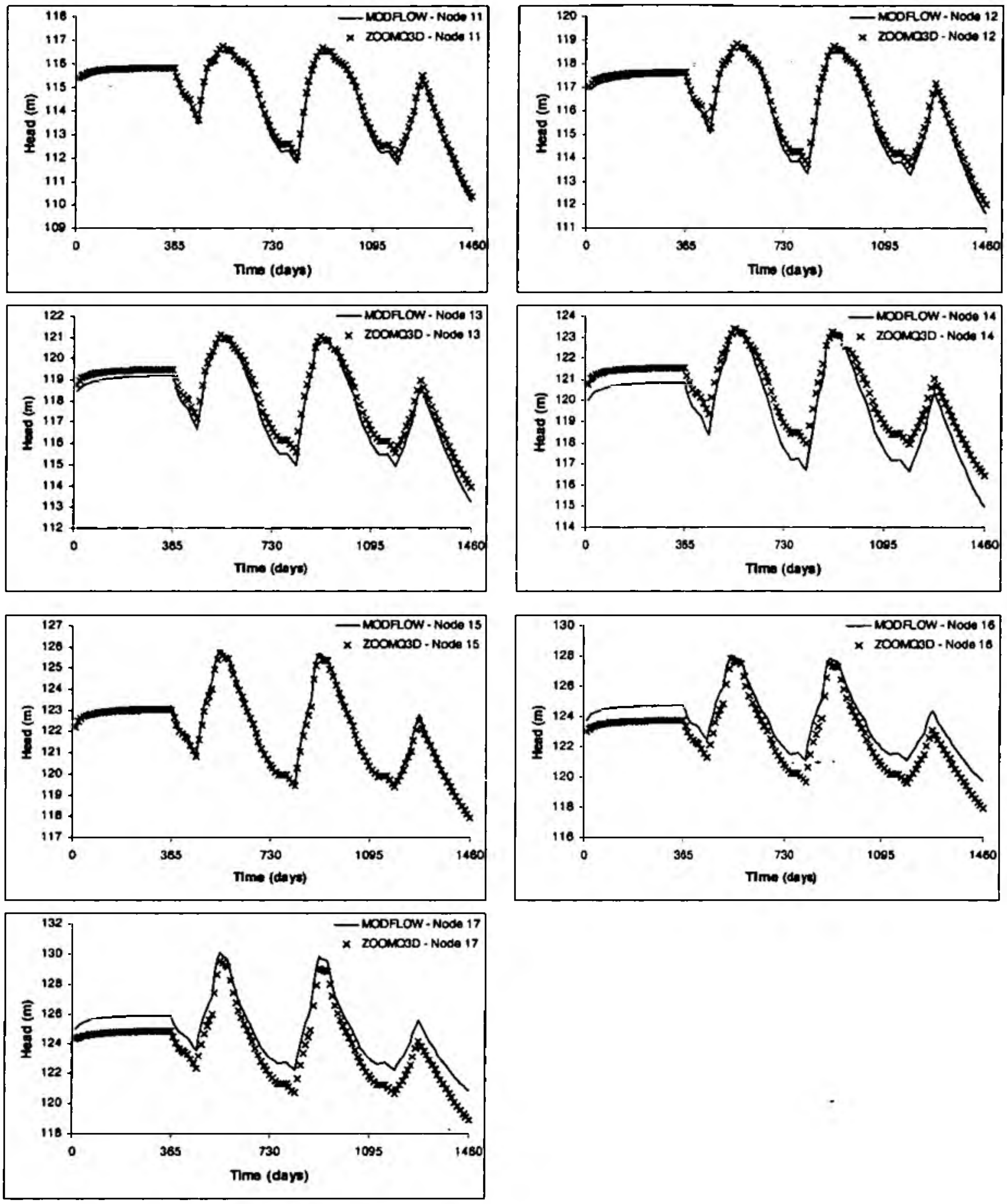


Figure 24 Simulated groundwater heads long river channel in Test 3b

(Node 17 at the upstream end of the river)

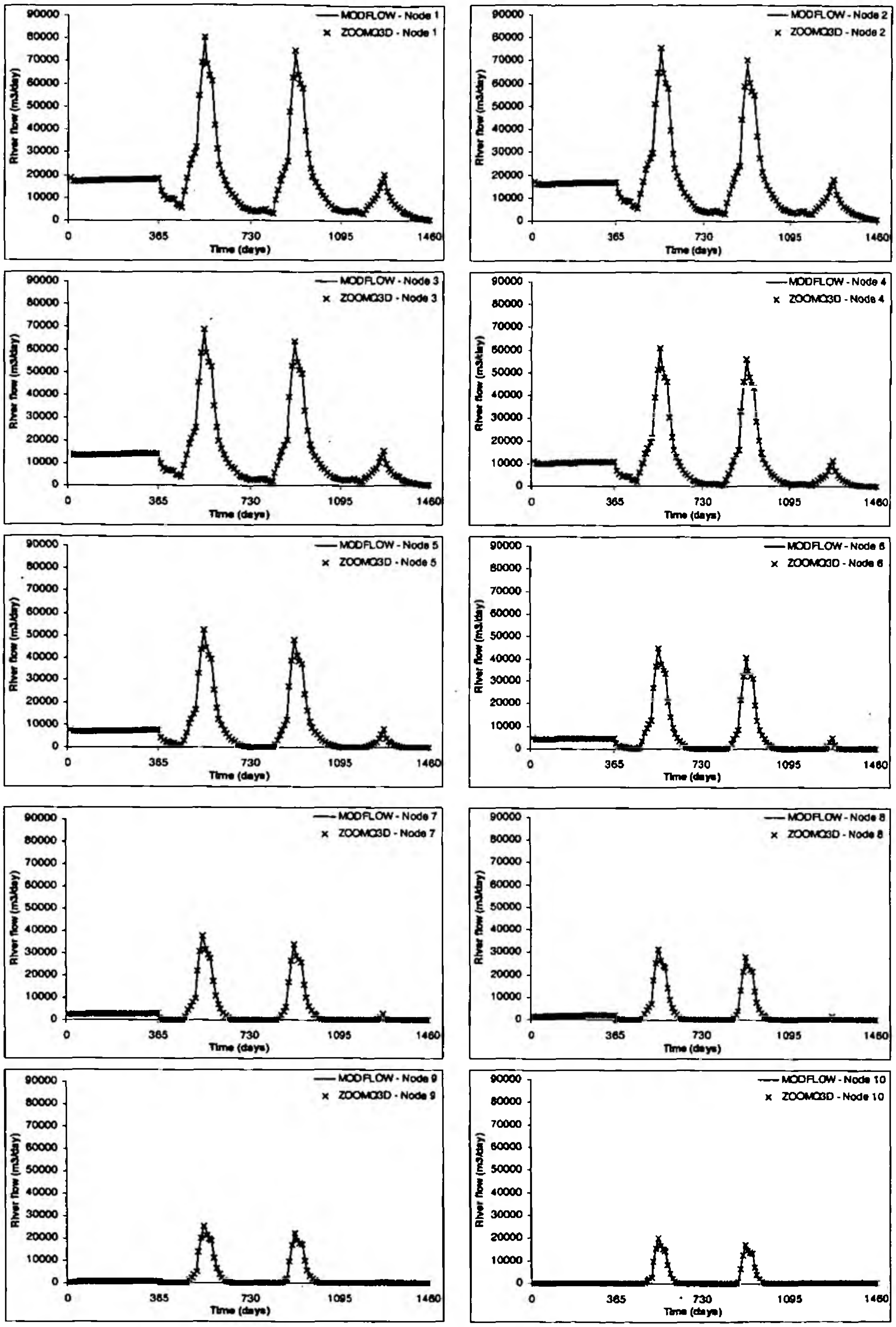


Figure 25 Simulated river flows in Test 3b

(Node 1 at the downstream end of the river)

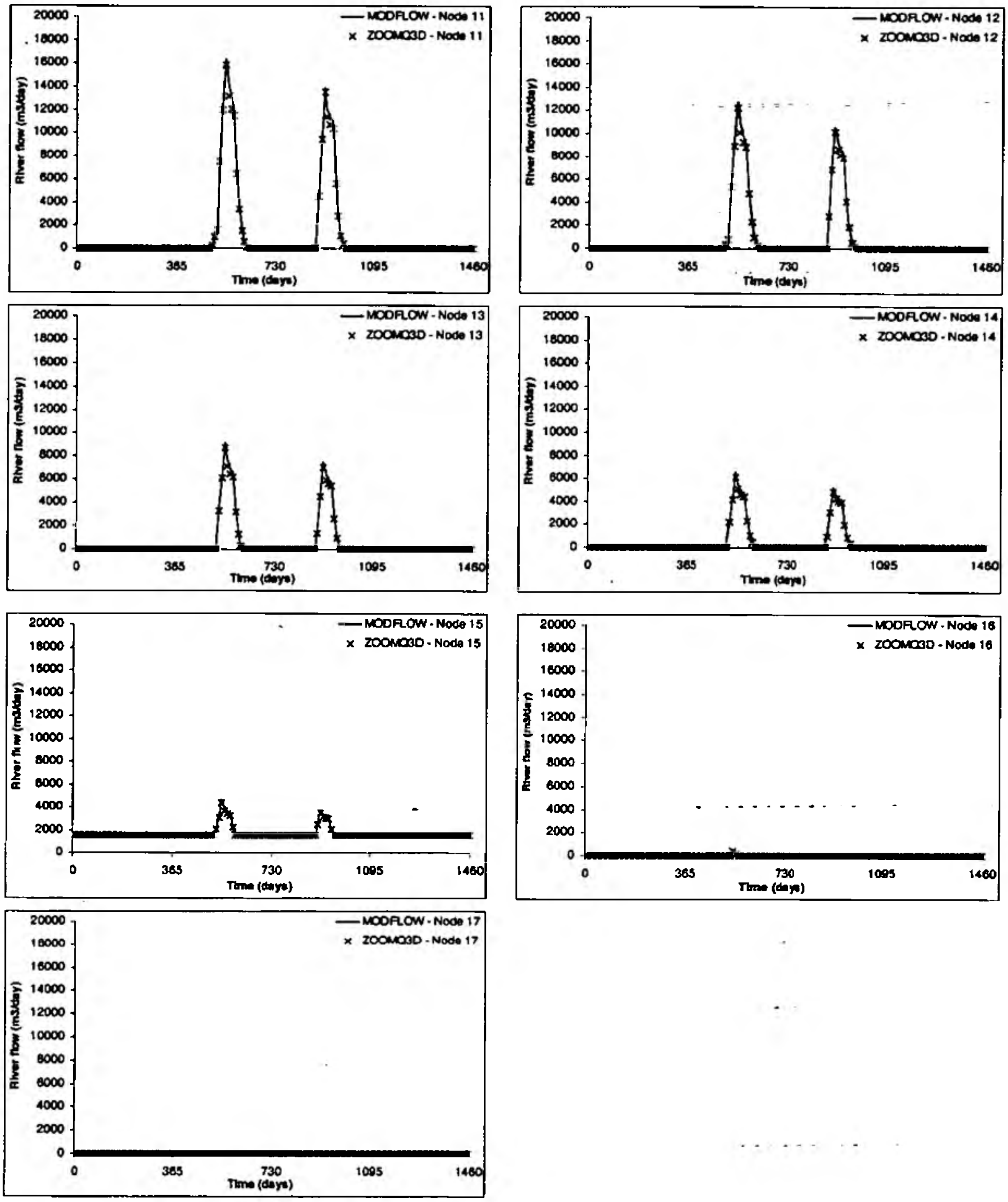


Figure 26 Simulated river flows in Test 3b

(Node 17 at the upstream end of the river)

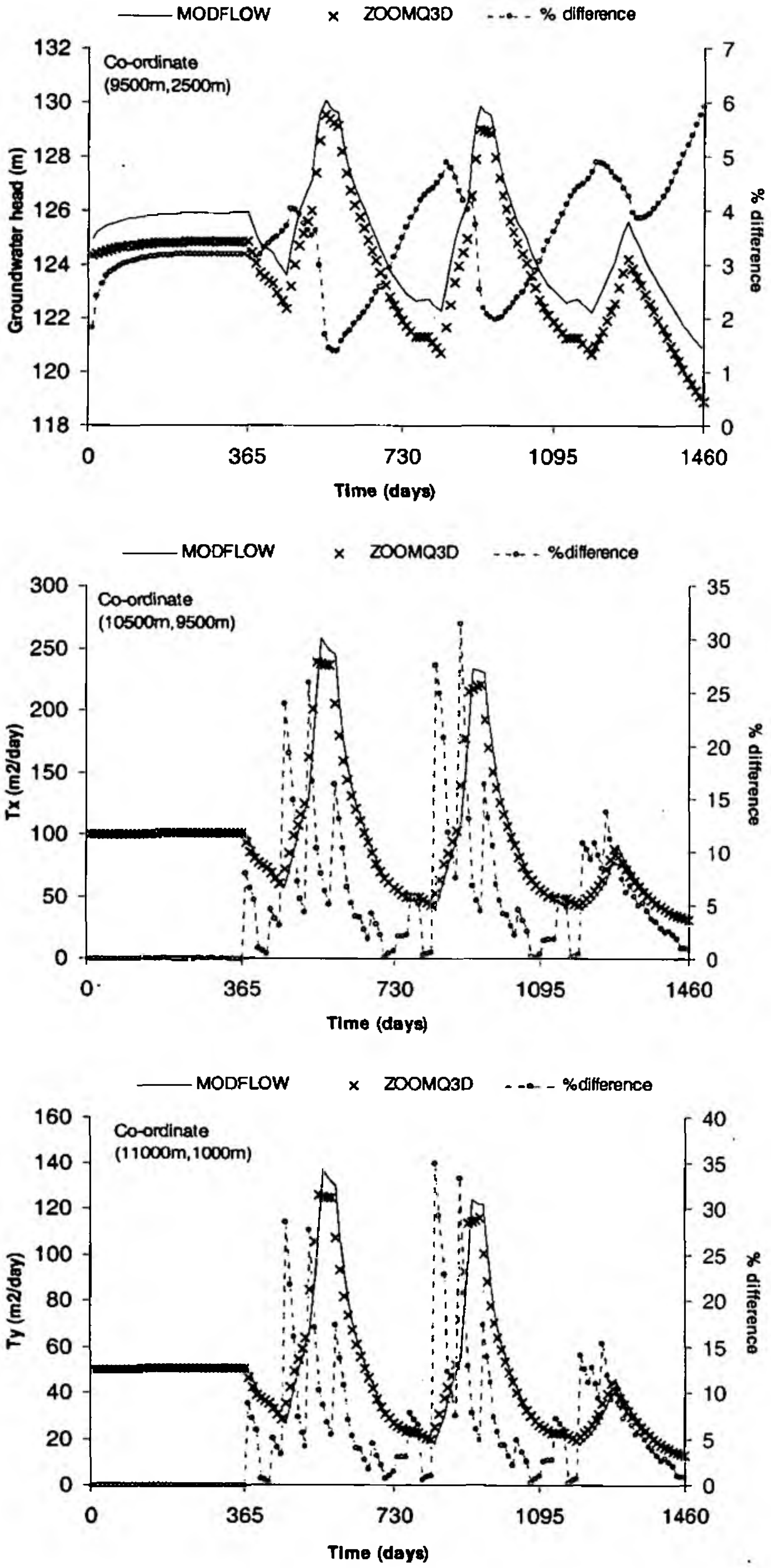


Figure 27 Simulated groundwater head and transmissivity hydrographs at the nodes of the Test 3b model that exhibit the greatest differences between ZOOMQ3D and MODFLOW

6.4.3 Test 3c

In this test, the ZOOMQ3D model is identical to the model used in Test 3b. The MODFLOW model is also the same except for one modification to the method of updating transmissivity. MODFLOW is made to update transmissivity in the same way as ZOOMQ3D by specifying that the model uses the latest value of groundwater head for its calculation. Dry river nodes are allowed to re-wet immediately after the groundwater head rises above the river bed in both models. ZOOMQ3D performs these tasks using time-step cycling. Transmissivity is a function of the average groundwater head at the end of the last two time-step cycles. In contrast, MODFLOW updates transmissivity and checks for the re-wetting of dry river nodes between the iterations of the numerical solution algorithm. The transmissivity in the MODFLOW model is updated using the latest value of groundwater head calculated during the solution process instead of the head at the beginning of the time-step. The previous two tests, Test 3a and 3b, have illustrated some of the differences between ZOOMQ3D and MODFLOW when simulating ephemeral rivers and unconfined aquifers. The discrepancies between the simulated results in these previous tests are due to differences in the numerical algorithms within the two codes. However, as stated above, these differences are removed in this test.

The comparison between the two models is shown in Figures 28 to 34. Again, in Figures 28 and 29 the groundwater hydrographs are plotted for the seventeen nodes along the river. In Figures 30 and 31 the flow hydrographs are shown for the seventeen river nodes. These four figures show good agreement by the two models. Figure 32 shows the simulated groundwater head and transmissivity hydrographs at the nodes exhibiting the poorest agreement between the two models. Acceptance criterion 2, relating to the comparison of groundwater head, is not violated during the simulation. Acceptance criterion 1, relating to the comparison of transmissivity, is violated only twice during the simulation at these poorest agreeing nodes. The time-variant global flow balance terms are shown in Figure 33. Again there is good agreement between the two models though the exact magnitude of the differences is difficult to infer from the figure. Consequently, the differences in the simulated global flow balance. terms are plotted in Figure 34. Predefined global flows, such as abstraction and recharge are identical in the two models and therefore are not plotted in the figure. Figure 34 shows that the storage change global flow balance term is violated only five times during the simulation. A summary of the differences between the two models is presented in Table 10.

Table 10 Summary of acceptance criteria values for Test 3c model

Acceptance criterion		Maximum difference	Criterion value	Total number of failures	Average number of failures per time-step
1. Groundwater head		0.27 % at (8000 m, 4000 m)	0.5%	0	0
(% of head variation)		≈ 0.09 m			
2. Transmissivity	**Tx**	2.0 % at (8000 m, 4000 m)	1.0%	2	0.014
		≈ 16.7 m^2/day			
	Ty	1.9 % at (8000 m, 4500 m)	1.0%	2	0.014
		≈ 16.8 m^2/day			
3. River flow		0.9 % at river node 14	2.0%	0	0
(% of max accreted flow)		≈ 274.9 m^3/day			
4. Global flows		0.67 % (storage change)	0.5%	5	0.035

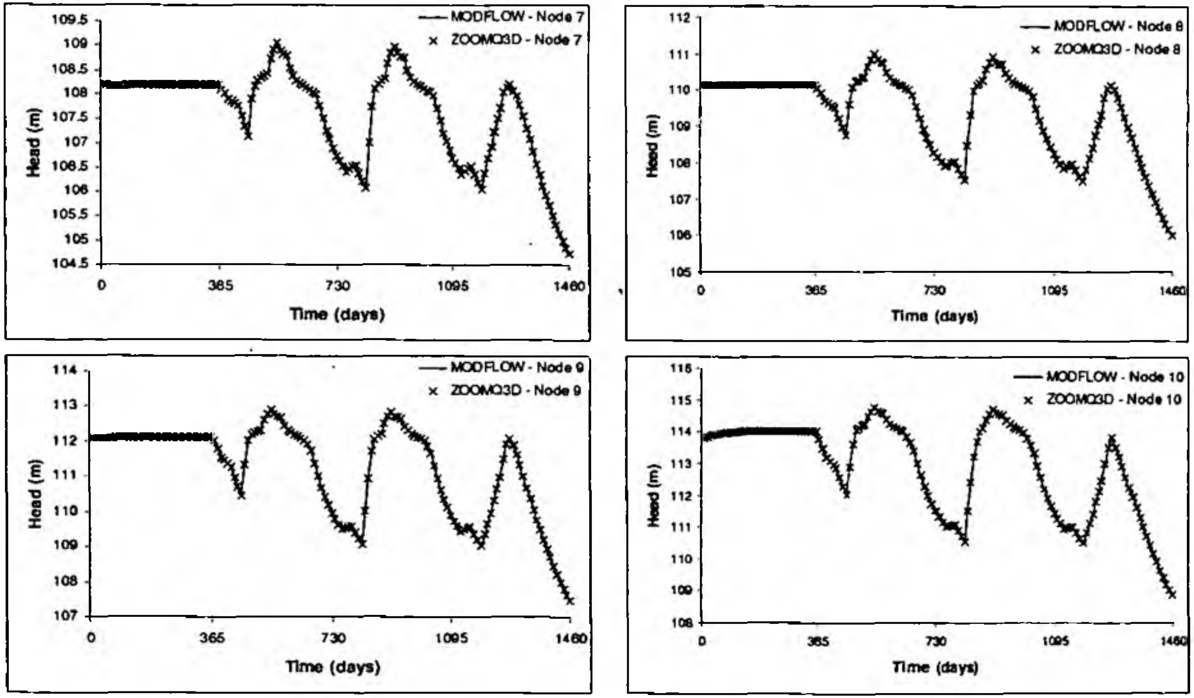
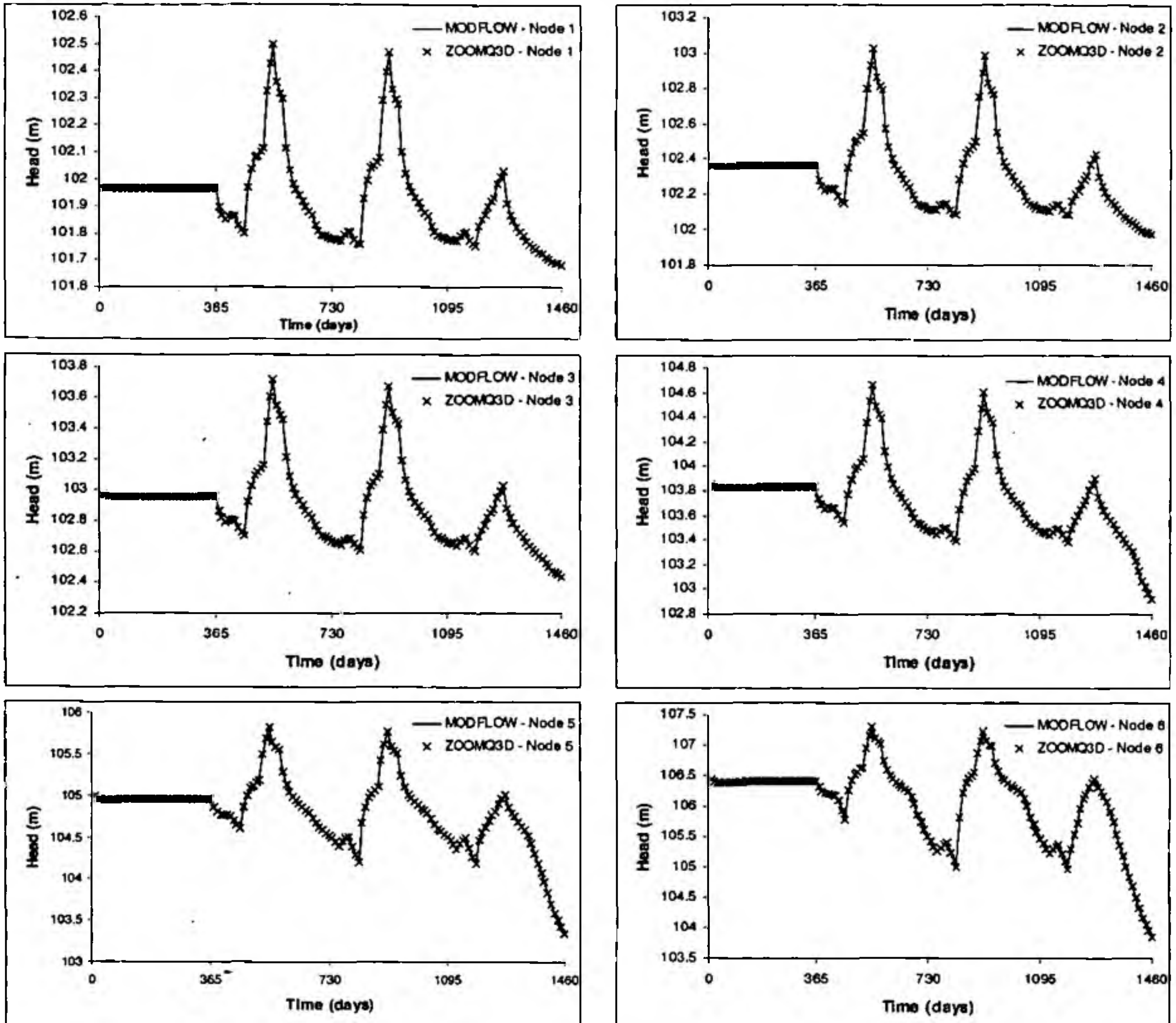


Figure 28 Simulated groundwater heads long river channel in Test 3c

(Node 1 at the downstream end of the river)


MODFLOW - Node 1
ZOOMQ3D - Node 1
Head (m)
Time (days)
MODFLOW - Node 2
ZOOMQ3D - Node 2
Head (m)
Time (days)
MODFLOW - Node 3
ZOOMQ3D - Node 3
Head (m)
Time (days)
MODFLOW - Node 4
ZOOMQ3D - Node 4
Head (m)
Time (days)
MODFLOW - Node 5
ZOOMQ3D - Node 5
Head (m)
Time (days)
MODFLOW - Node 6
ZOOMQ3D - Node 6
Head (m)
Time (days)

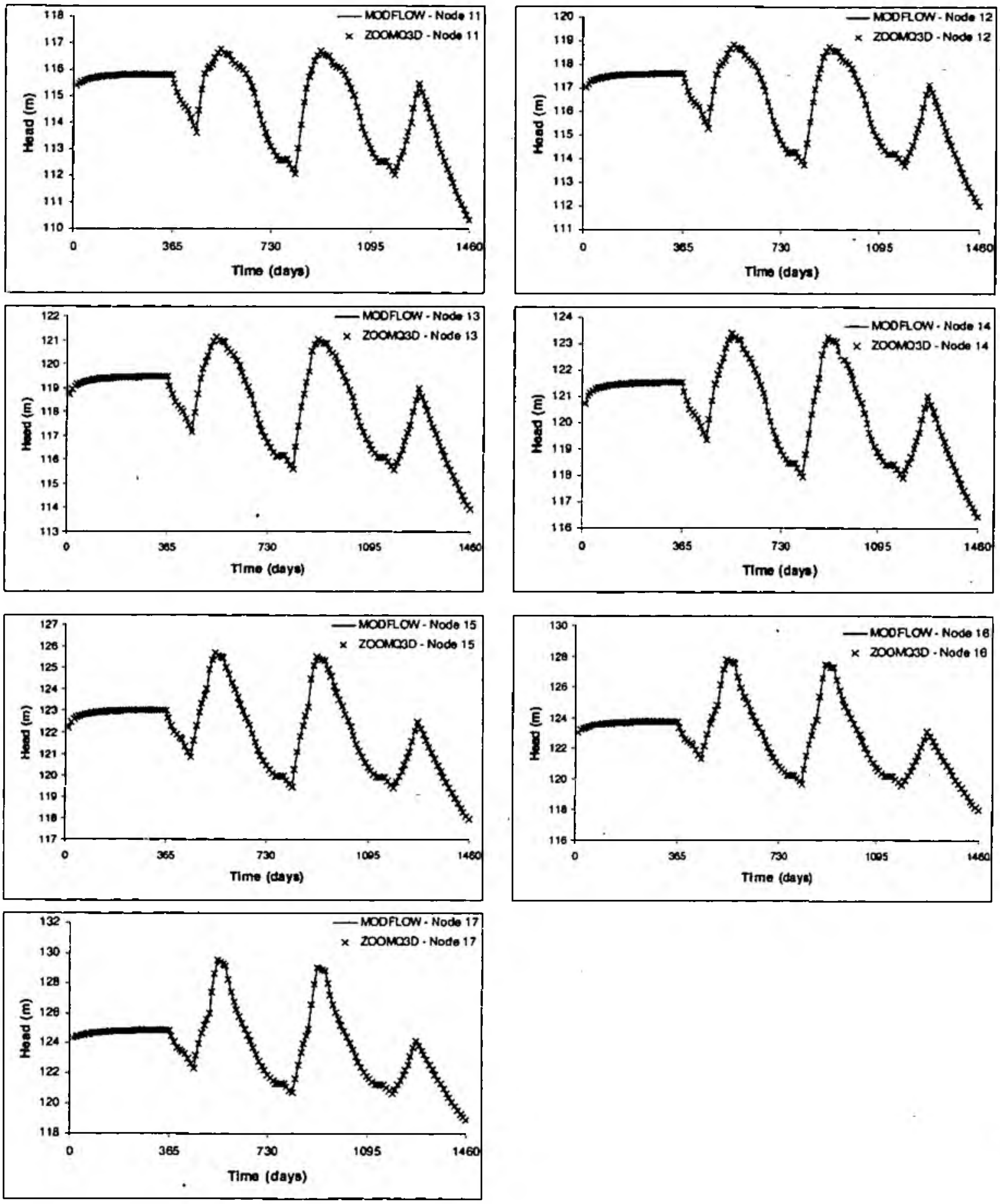


Figure 29 Simulated groundwater heads long river channel in Test 3c

(Node 17 at the upstream end of the river)

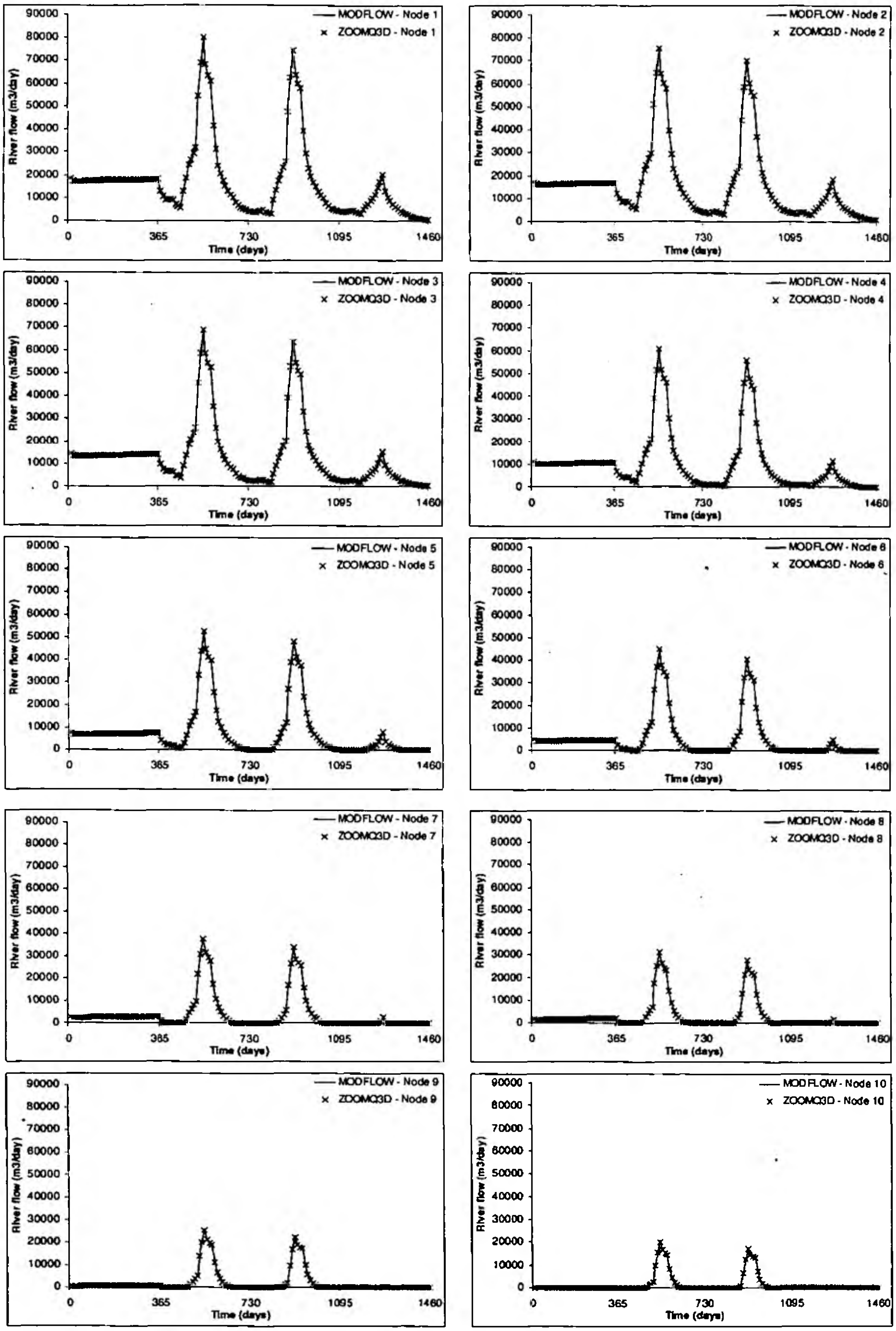


Figure 30 Simulated river flows in Test 3c

(Node 1 at the downstream end of the river)

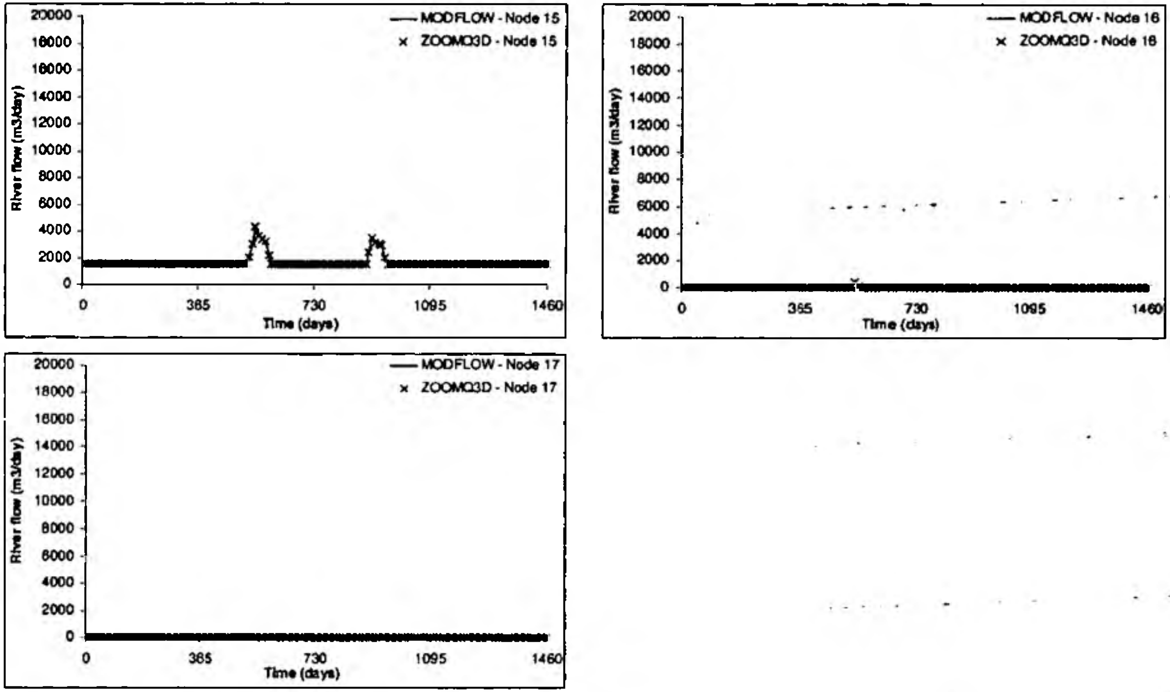
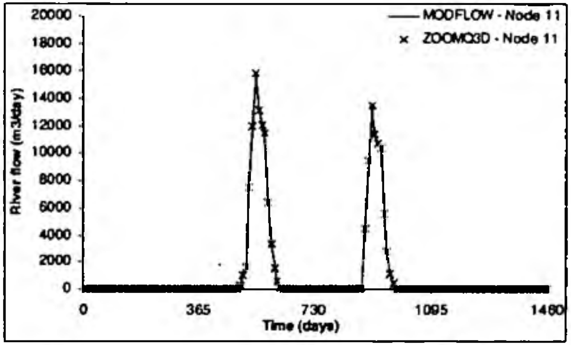
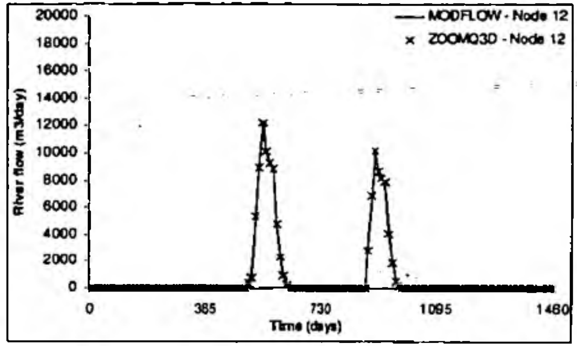


Figure 31 Simulated river flows in Test 3c

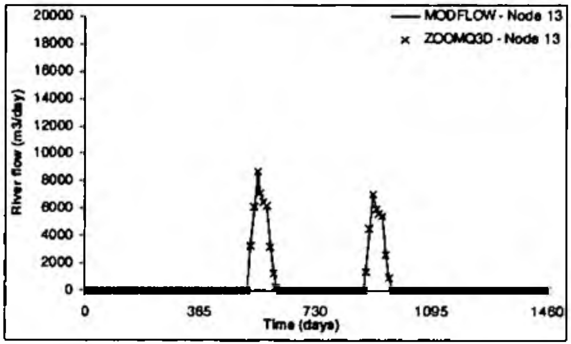
(Node 17 at the upstream end of the river)



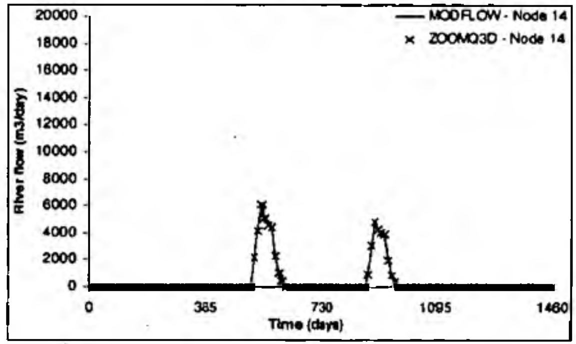
MODFLOW - Node 11
ZOOMQ3D - Node 11
River flow (m3/day)
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
0
365
730
1095
1460
Time (days)



MODFLOW - Node 12
ZOOMQ3D - Node 12
River flow (m3/day)
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
0
365
730
1095
1460
Time (days)



MODFLOW - Node 13
ZOOMQ3D - Node 13
River flow (m3/day)
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
0
365
730
1095
1460
Time (days)



MODFLOW - Node 14
ZOOMQ3D - Node 14
River flow (m3/day)
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
0
365
730
1095
1460
Time (days)

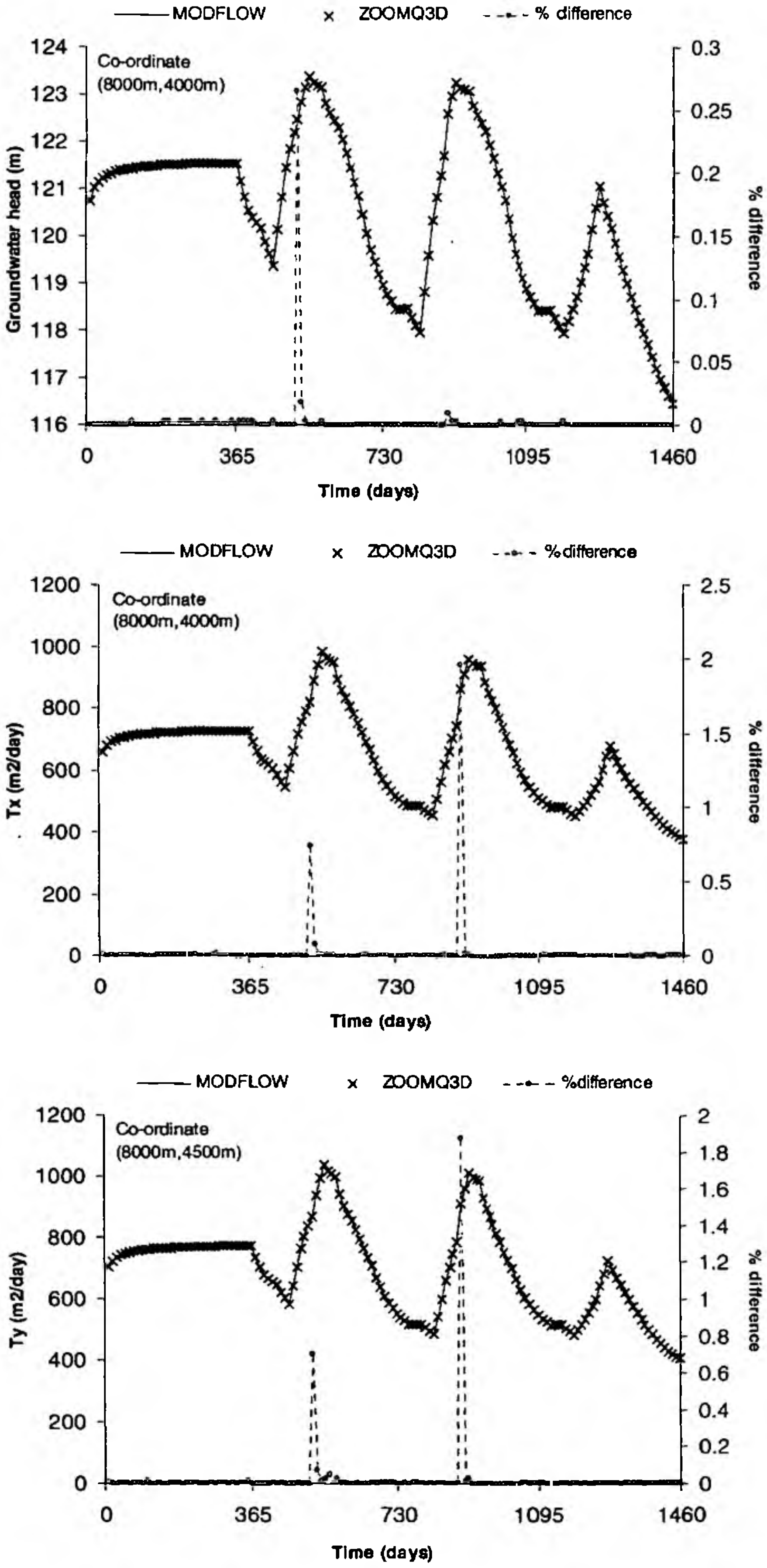


Figure 32 Simulated groundwater head and transmissivity hydrographs at the nodes of the Test 3c model that exhibit the greatest differences between ZOOMQ3D and MODFLOW

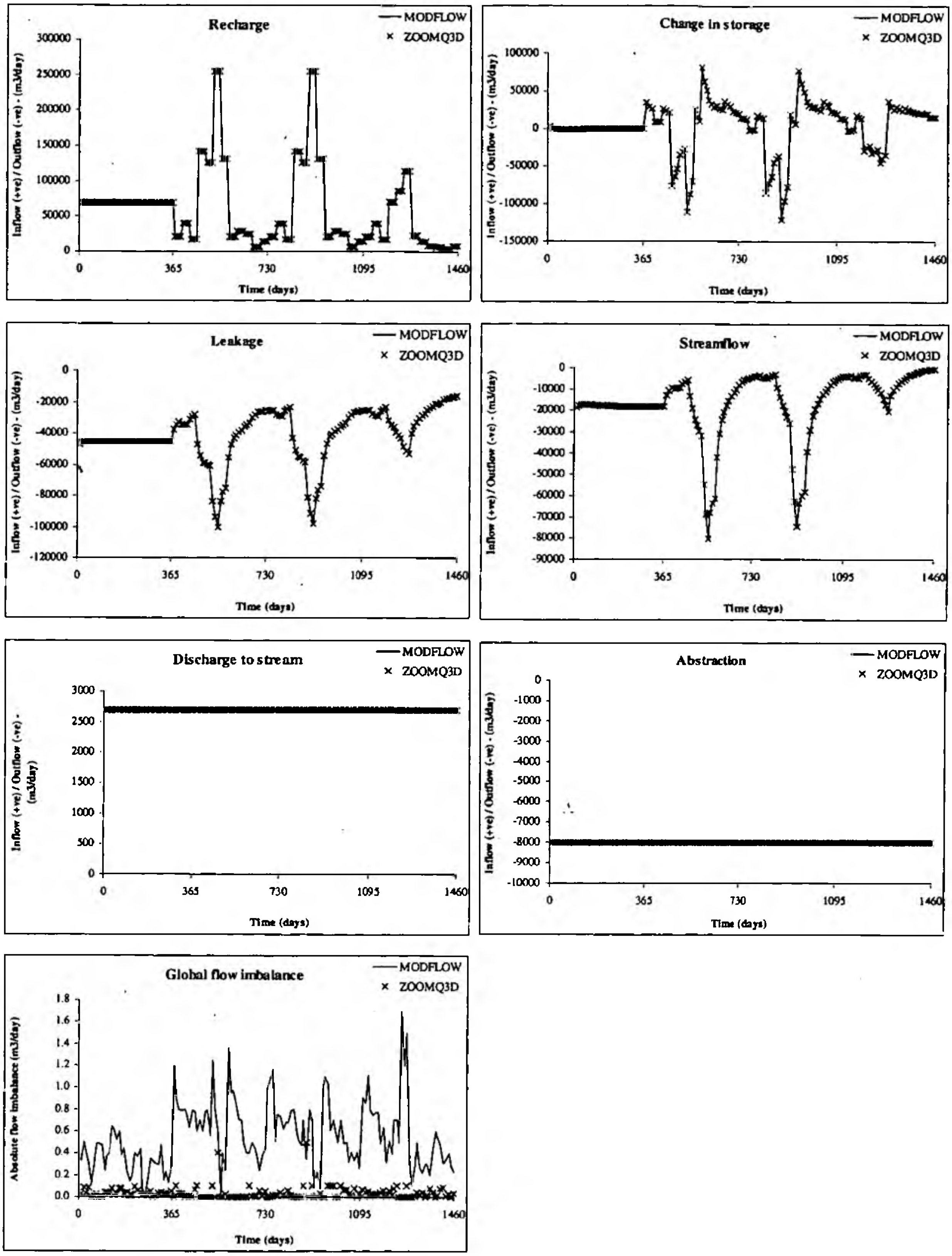


Figure 33 Simulated global flows for each feature of the Test 3c model

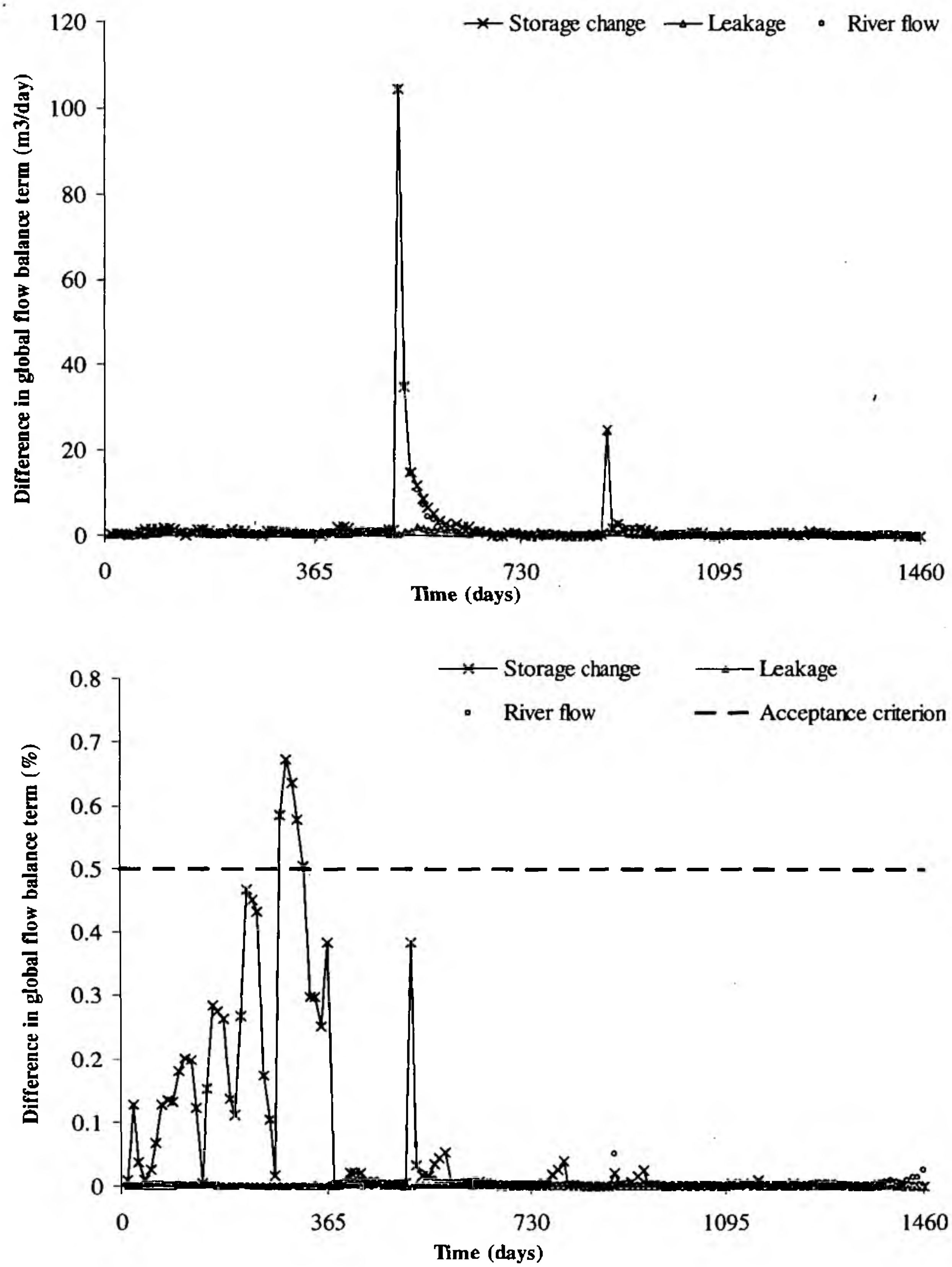


Figure 34 Absolute and percentage differences in global flows between the Test 3c ZOOMQ3D and MODFLOW models

6.5 TEST4: FLOW TO A WELL IN A ONE LAYER REFINED GRID MODEL

To validate the applicability of VKD in a model with a locally refined grid, two test models are constructed. The first of these, the model used in this test, is shown in Figure 35. The model is 10 km square and has a uniform 1 km square base mesh. The coarse base grid is refined in the central 4 km square, to a mesh of 200 m square cells, in one refinement step. Recharge is applied uniformly across the aquifer at a constant rate of 0.1 mm/day and all model boundaries are impermeable. VKD parameters are uniform throughout the model. The elevation of the base of the aquifer is specified as 0 m. Hydraulic conductivity is 10 m/day below an elevation of 150 m. Above this level, hydraulic conductivity increases linearly with elevation by 0.5 m/day per metre, i.e. VKDGrad is 0.5. The storage coefficient is uniform throughout the aquifer and is 0.01. The model simulates a four-year period starting from a flat water table 175 m above the base of the aquifer. A well located at the centre of the model pumps groundwater from the aquifer at varying rates during the simulation. These pumping rates are listed in Table 11.

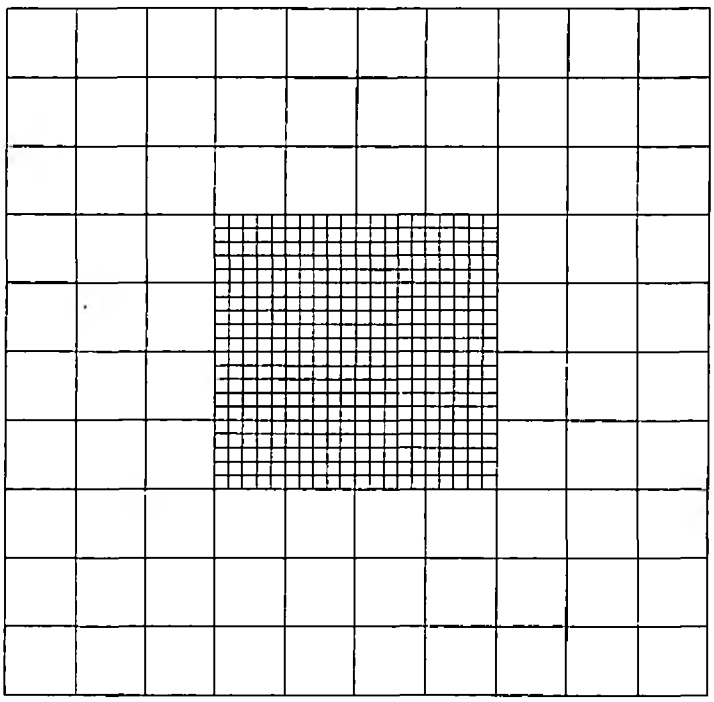


Figure 35 Test 4 refined grid model

Table 11 Pumping rates for Test 4 model

	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Year 1	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
Year 2	9.75	9.5	9.25	9.0	8.75	8.5	8.25	8.0	8.25	8.5	8.75	9.0
Year 3	9.25	9.5	9.75	10.0	10.25	10.5	10.75	11.0	11.25	11.5	11.75	12.0
Year 4	11.75	11.5	11.25	11.0	10.75	10.5	10.25	10.0	10.0	10.0	10.0	10.0

To examine if there any problems associated with the application of VKD profiles in locally refined grid models, this model is compared to one with a uniform fine mesh across the whole of the aquifer. The two models are identical except for the finite difference grid. The fine grid model mesh is 200 m square, which is the same as the mesh at the centre of the refined grid model. The two models are compared by examining the groundwater head hydrographs at coincident nodes across the centre of the aquifer along the line y=5000 m. These comparisons are shown in Figure 36 and Figure 37. The two models simulate very similar groundwater heads during the four-year period. The difference between the simulated groundwater heads for corresponding groundwater hydrographs is plotted as a percentage of the maximum variation in groundwater head across the aquifer (maximum groundwater head minus minimum groundwater head). The largest difference between the two models is 0.25% at co-ordinate (3000 m, 5000 m), which is equivalent to an absolute difference in head of 12 mm. This difference is considered small and indicates that the use of VKD is acceptable in locally refined grid models. However, to confirm this finding a second locally refined grid model is constructed. This is described in the next section.

6.6 TEST 5: FLOW TO A WELL IN A TWO LAYER REFINED GRID MODEL

In this test, as in Test 4, a refined grid model is compared to a fine grid model. VKD is implemented in both models which are identical to those described in the previous test except for the fact that two layers are used instead of one. The base of the top layer is fifty metres above the base of the bottom layer which is taken as the datum. The well is specified to abstract water from the bottom layer only. However, the pumping rates are identical to those listed in Table 11. The vertical conductance is uniform across the aquifer and is 10^{-6} day^{-1}. Groundwater head is monitored in the top layer of both models along the line y = 5000 m.

The fine and refined grid models simulate very similar variations in groundwater head over the four-year period. The comparisons are shown in Figure 38 and Figure 39. The maximum difference between corresponding groundwater hydrographs is 0.247% at co-ordinate (3000 m, 5000 m), which is equivalent to an absolute head difference of 26 mm. Again this is considered small and consequently it is concluded that the implementation of VKD in models using local grid refinement is acceptable.

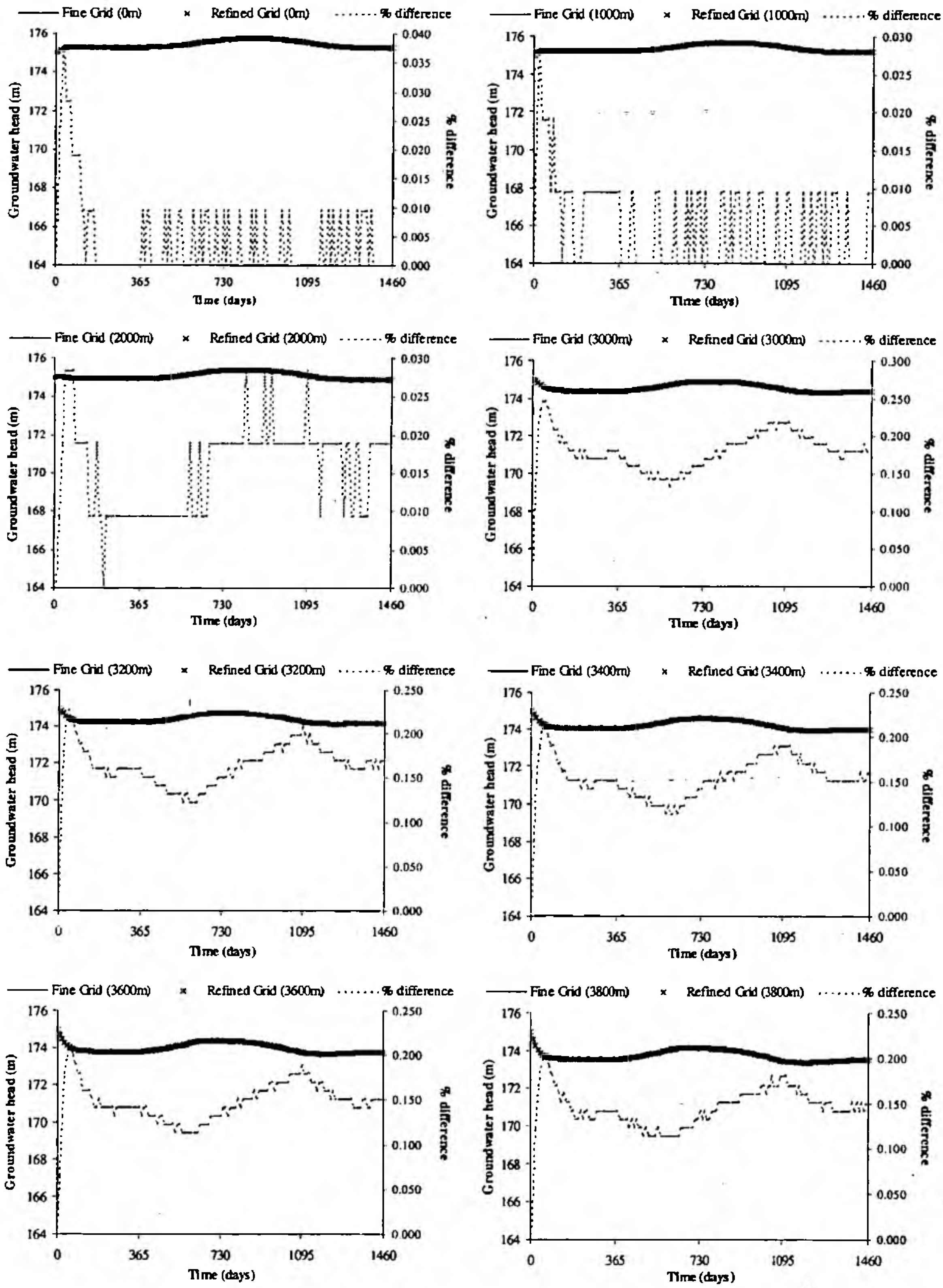


Figure 36 Groundwater hydrographs for Test 4 refined and fine grid models Comparison along line y=5000 m, x co-ordinate shown on graphs.

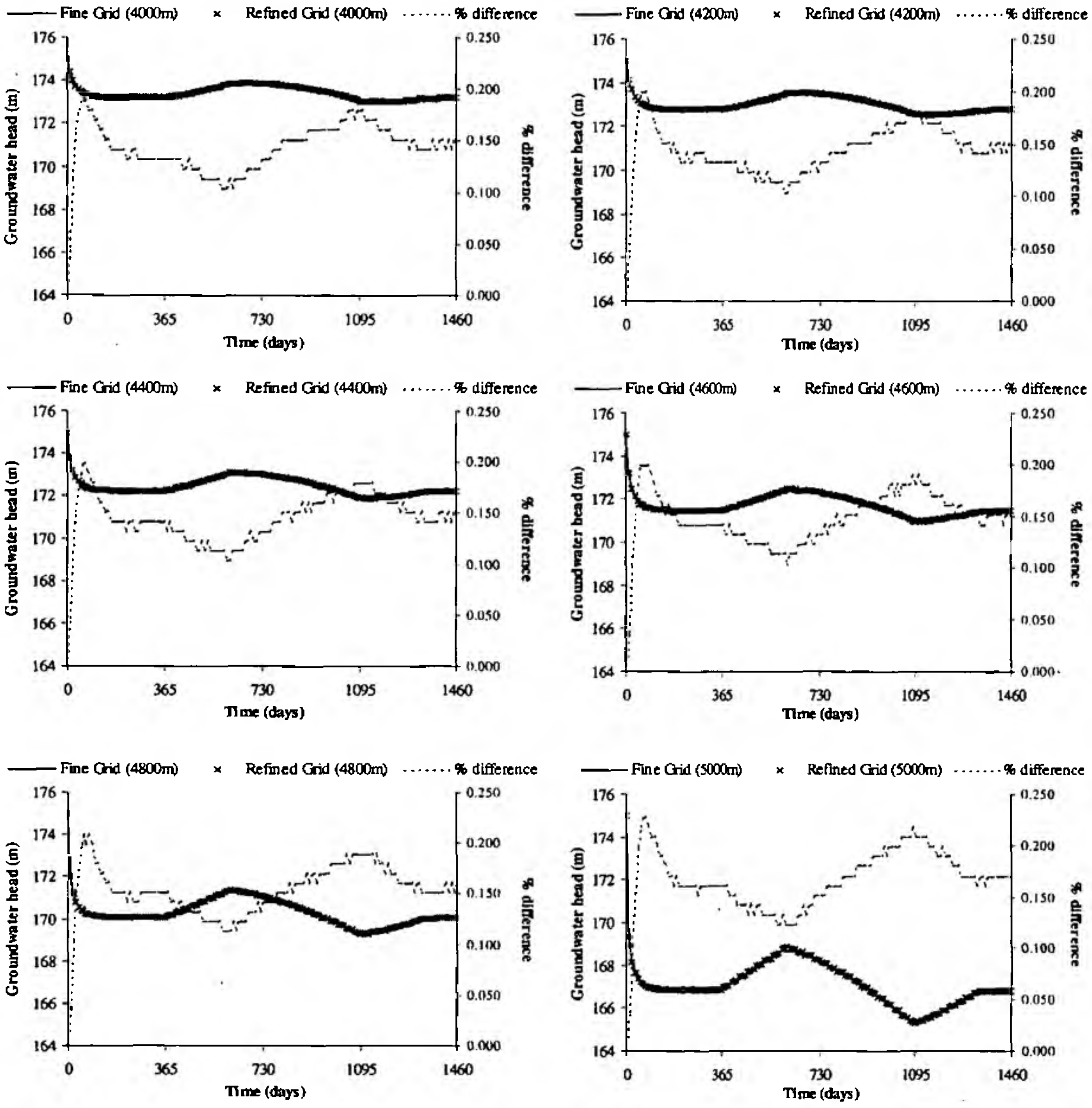


Figure 37 Groundwater hydrographs for Test 4 refined and fine grid models Comparison along line y=5000 m, x co-ordinate shown on graphs.

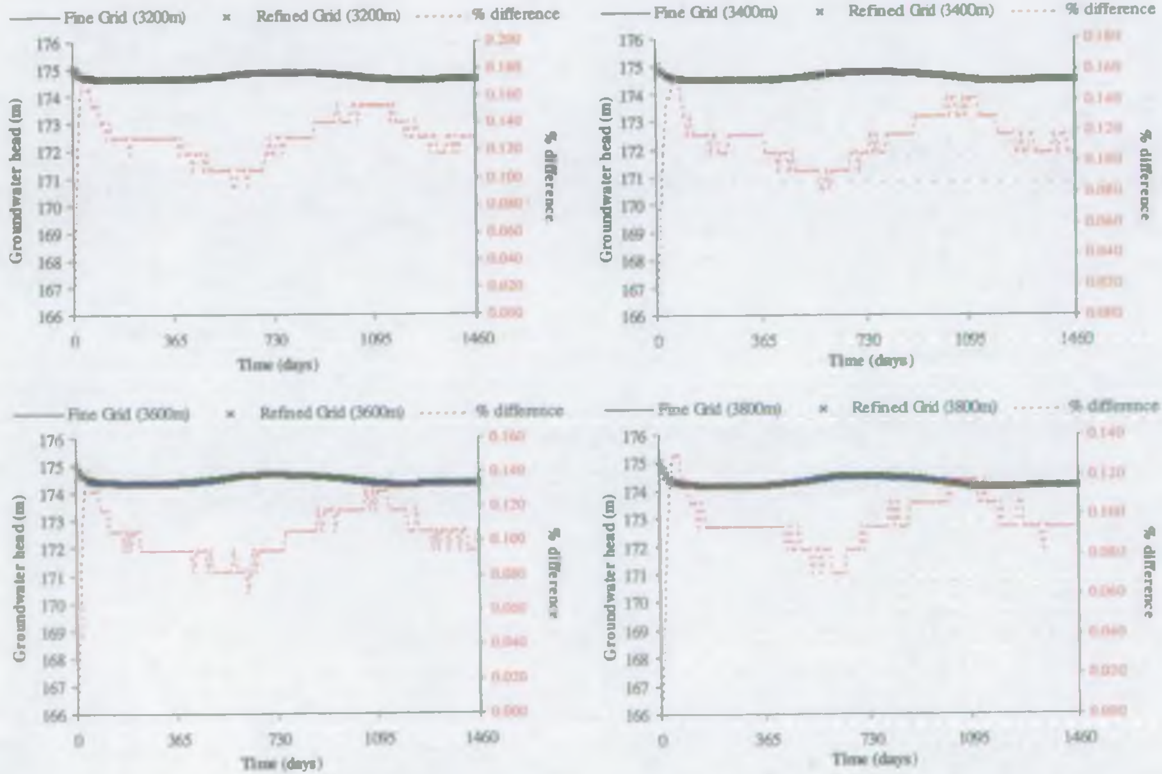
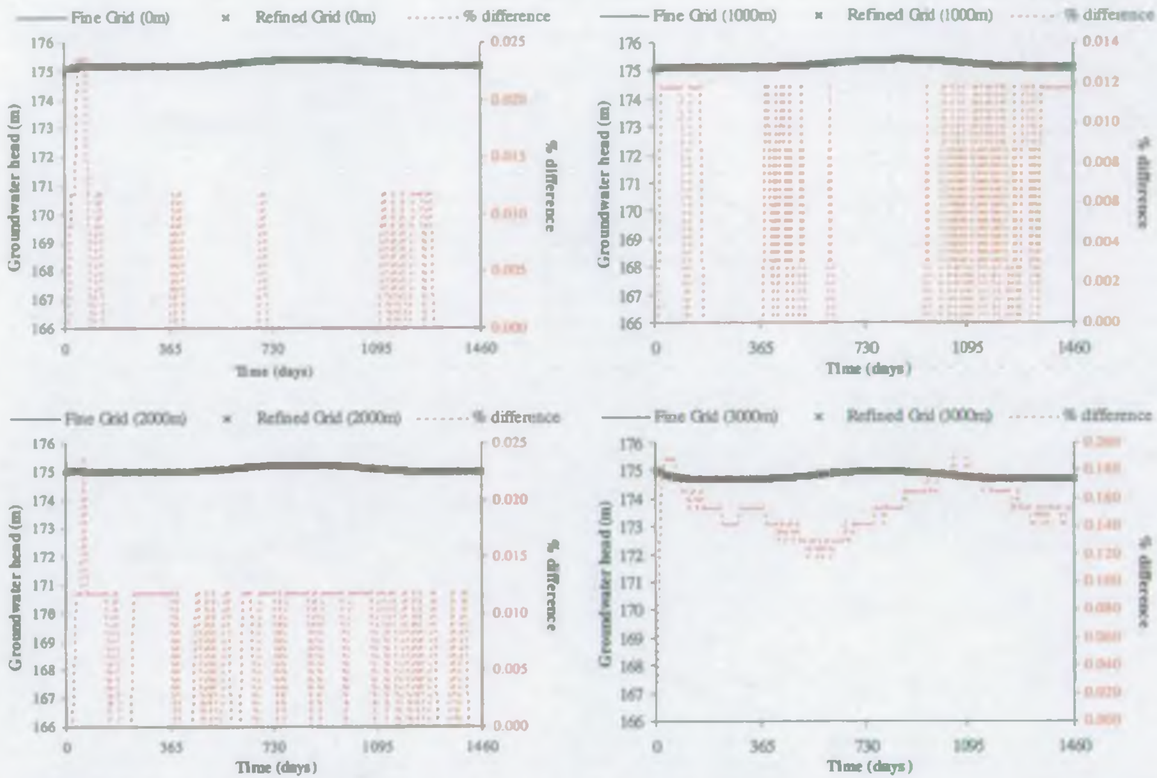


Figure 38 Groundwater hydrographs for Test 5 refined and fine grid models Comparison along line y=5000 m, x co-ordinate shown on graphs.


Fine Grid (0m)
Refined Grid (0m)
% difference
Groundwater head (m)
% difference
Time (days)
Fine Grid (1000m)
Refined Grid (1000m)
% difference
Groundwater head (m)
% difference
Time (days)
Fine Grid (2000m)
Refined Grid (2000m)
% difference
Groundwater head (m)
% difference
Time (days)
Fine Grid (3000m)
Refined Grid (3000m)
% difference
Groundwater head (m)
% difference
Time (days)

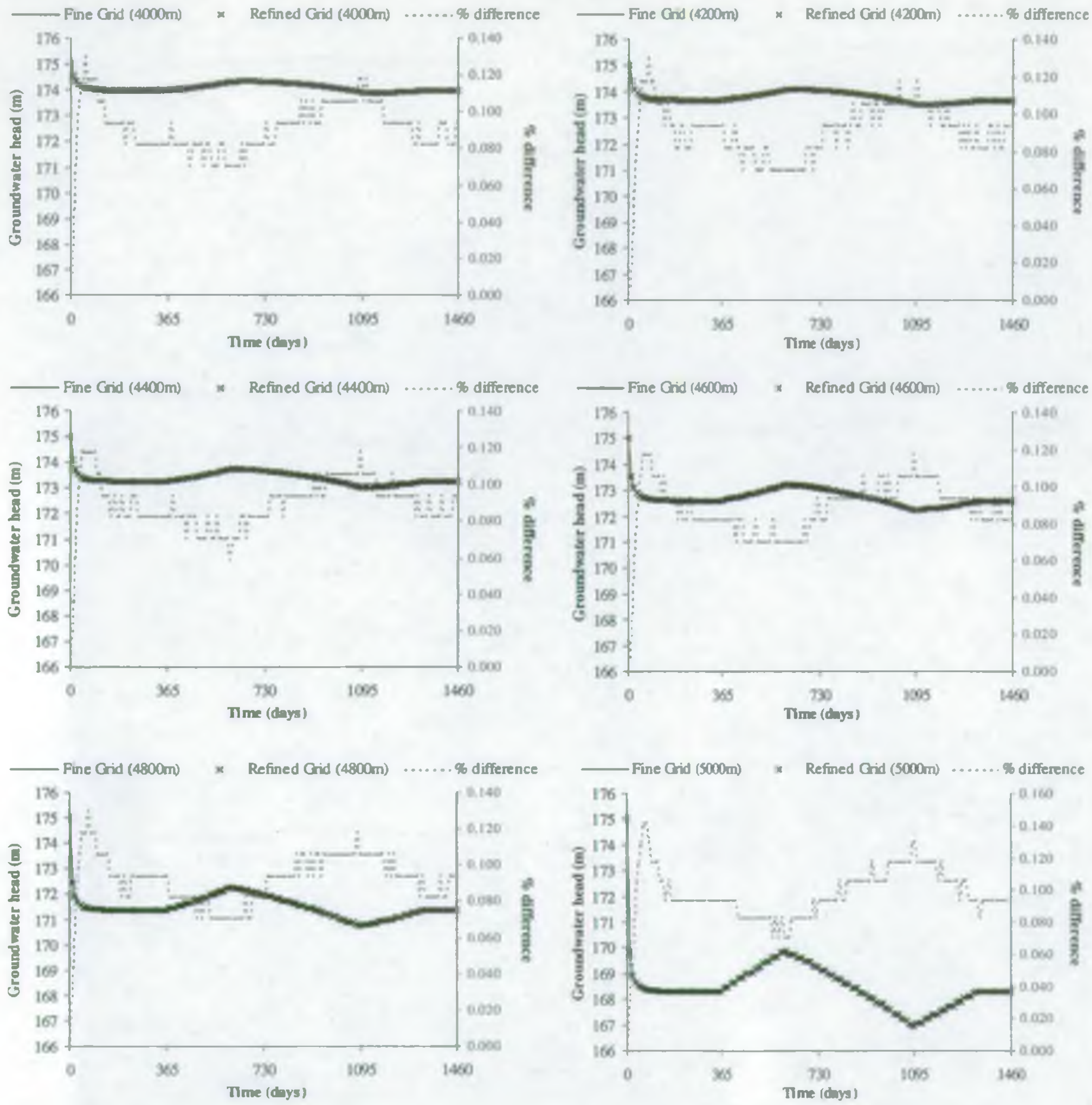


Figure 39 Groundwater hydrographs for Test 5 refined and fine grid models
Comparison along line y=5000 m, x co-ordinate shown on graphs.

7 Conclusions

The representation of the variation of hydraulic conductivity with depth (VKD) has been successfully implemented in ZOOMQ3D. The development and incorporation of VKD in the model code has been a relatively straightforward procedure and was achieved within approximately five man-days. A number of tests were then performed to validate the modified code.

One additional class has been added to the framework of objects on which ZOOMQ3D is built. This class encapsulates the description of the vertical variation of hydraulic conductivity with depth in the aquifer. A relatively simple, but nevertheless important, representation of the variation of hydraulic conductivity has been implemented in the model; the linear increase in hydraulic conductivity with elevation above a specified point. The use of this representation of hydraulic conductivity is often important when simulating limestone and, in particular Chalk aquifers, where higher conductivities are generally associated with the zone of fluctuation of the water table.

Though the representation of the hydraulic conductivity profile is not complex, because of its encapsulation in objects, modification of the profiles' shape should be a relatively simple task. The more significant problem associated with the application of physically realistic conductivity profiles will be the storage, management and transfer of *data* into the model code.

Testing of the modified ZOOMQ3D model has shown that it has been incorporated correctly in the code. Tests have included the application of local grid refinement in models using VKD and these have indicated that their conjunctive use is acceptable. However, greater confidence in the simultaneous use of these two model features will and should be gained by the further application of the model to real problems.

ZOOMQ3D has been benchmarked against the modified MODFLOW code using an example model presented by Environment Agency (1999). The two models have produced very similar results during this validation procedure, however, this process has highlighted that the user must be aware of the subtle differences between MODFLOW and ZOOMQ3D. These relate to the updating of the finite difference equations over time. MODFLOW allows the modification of the coefficients of the finite difference equations *during* its iterative solution procedures. Consequently transmissivity can be updated and dry river nodes allowed to re-wet as the groundwater head changes *during* the solution. Whilst this technique has some benefits it can prevent certain models from converging. In contrast ZOOMQ3D does not allow the finite difference equations to be modified whilst the solution is being calculated. Instead, unconfined aquifers and ephemeral rivers are simulated using a cyclical procedure, in which the solution for the time-step is repeated a number of times.

With regard to the future development of the representation of VKD in ZOOMQ3D, this should occur in parallel to the application of the model to real aquifers and its comparison to other MODFLOW models. As with this project the further development of the model should continue to employ the expertise of each of the collaborating organisations. This process may involve a more fundamental examination of the way conceptual models of Chalk groundwater flow are transferred into numerical models.

Appendix 1 Test 1, 2 and 3 model VKD parameters

Aquifer base elevation (m) by row and column

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
21	36.617	36.585	36.490	40.305	44.143	48.027	51.965	55.958	60.003	64.090	68.214	72.365	76.536	80.720	84.911	89.103	93.289	97.463	101.620	105.730	109.780	113.710	117.240
20	36.611	36.579	36.483	40.281	44.108	47.988	51.926	55.923	59.972	64.065	68.193	72.348	76.523	80.710	84.903	89.097	93.285	97.460	101.610	105.730	109.780	113.710	117.240
19	36.593	36.559	36.460	40.201	43.996	47.866	51.809	55.817	59.881	63.989	68.131	72.299	76.484	80.680	84.881	89.080	93.273	97.451	101.610	105.730	109.780	113.700	117.240
18	36.566	36.528	36.417	40.038	43.784	47.647	51.605	55.638	59.729	63.864	68.030	72.219	76.423	80.633	84.846	89.054	93.254	97.437	101.600	105.720	109.780	113.700	117.240
17	36.539	36.494	36.354	39.717	43.428	47.309	51.306	55.384	59.519	63.694	67.897	72.115	76.343	80.574	84.801	89.022	93.231	97.422	101.590	105.710	109.770	113.700	117.230
16	36.525	36.479	36.337	39.680	42.872	46.835	50.910	55.059	59.258	63.489	67.737	71.994	76.253	80.507	84.753	88.988	93.208	97.406	101.580	105.710	109.770	113.700	117.230
15	36.526	36.482	36.348	39.738	43.036	46.232	50.427	54.675	58.958	63.259	67.565	71.867	76.160	80.441	84.708	88.958	93.188	97.395	101.570	105.700	109.770	113.700	117.240
14	36.540	36.498	36.372	39.839	43.245	46.590	49.887	54.252	58.638	63.023	67.395	71.747	76.077	80.386	84.672	88.937	93.177	97.391	101.570	105.710	109.780	113.710	117.240
13	36.562	36.522	36.402	39.954	43.466	46.938	50.383	53.810	58.325	62.806	67.247	71.650	76.016	80.350	84.654	88.930	93.179	97.399	101.580	105.720	109.790	113.720	117.260
12	36.587	36.549	36.433	40.071	43.680	47.266	50.843	54.428	58.057	62.639	67.148	71.595	75.991	80.344	84.660	88.944	93.197	97.419	101.610	105.750	109.820	113.750	117.280
11	36.614	36.576	36.463	40.180	43.877	47.562	51.249	54.956	58.714	62.564	67.121	71.600	76.015	80.377	84.697	88.981	93.234	97.455	101.640	105.780	109.850	113.780	117.320
10	36.639	36.602	36.491	40.279	44.052	47.821	51.596	55.396	59.244	63.166	67.189	71.680	76.099	80.455	84.767	89.043	93.290	97.506	101.690	105.820	109.890	113.820	117.360
9	36.662	36.625	36.515	40.365	44.203	48.040	51.887	55.757	59.669	63.642	67.695	71.844	76.251	80.580	84.869	89.128	93.362	97.569	101.740	105.880	109.940	113.870	117.400
8	36.683	36.646	36.536	40.438	44.330	48.223	52.125	56.049	60.008	64.016	68.087	72.236	76.485	80.745	84.995	89.230	93.447	97.642	101.810	105.930	109.990	113.920	117.450
7	36.700	36.663	36.553	40.498	44.435	48.372	52.318	56.282	60.274	64.305	68.384	72.517	76.703	80.912	85.127	89.337	93.536	97.719	101.880	105.990	110.050	113.970	117.510
6	36.714	36.677	36.567	40.546	44.519	48.491	52.470	56.464	60.481	64.528	68.610	72.731	76.886	81.064	85.251	89.440	93.623	97.793	101.940	106.050	110.100	114.020	117.560
5	36.725	36.689	36.578	40.584	44.584	48.583	52.587	56.604	60.639	64.697	68.781	72.894	77.033	81.190	85.359	89.532	93.701	97.861	102.000	106.110	110.150	114.070	117.600
4	36.734	36.697	36.586	40.612	44.632	48.651	52.674	56.707	60.754	64.820	68.907	73.016	77.145	81.290	85.446	89.607	93.766	97.918	102.050	106.150	110.190	114.110	117.640
3	36.740	36.703	36.592	40.632	44.666	48.698	52.734	56.777	60.833	64.904	68.993	73.099	77.223	81.361	85.509	89.662	93.815	97.960	102.090	106.190	110.230	114.140	117.670
2	36.744	36.706	36.595	40.644	44.686	48.726	52.769	56.819	60.879	64.953	69.043	73.149	77.270	81.404	85.547	89.696	93.845	97.986	102.110	106.210	110.250	114.160	117.690
1	36.745	36.708	36.596	40.647	44.692	48.735	52.780	56.832	60.894	64.969	69.059	73.165	77.285	81.418	85.560	89.707	93.855	97.995	102.120	106.220	110.250	114.170	117.700

VKD Zp elevation (m) by row and column

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
21	91.617	91.585	91.490	92.805	94.143	95.527	96.965	98.458	100.000	101.590	103.210	104.870	106.540	108.220	109.910	111.600	113.290	114.960	116.620	118.230	119.780	121.210	122.240
20	91.611	91.579	91.483	92.781	94.108	95.488	96.926	98.423	99.972	101.560	103.190	104.850	106.520	108.210	109.900	111.600	113.290	114.960	116.610	118.230	119.780	121.210	122.240
19	91.593	91.559	91.460	92.701	93.996	95.366	96.809	98.317	99.881	101.490	103.130	104.800	106.480	108.180	109.880	111.580	113.270	114.950	116.610	118.230	119.780	121.200	122.240
18	91.566	91.528	91.417	92.538	93.784	95.147	96.605	98.138	99.729	101.360	103.030	104.720	106.420	108.130	109.850	111.550	113.250	114.940	116.600	118.220	119.780	121.200	122.240
17	91.539	91.494	91.354	92.217	93.428	94.809	96.306	97.884	99.519	101.190	102.900	104.620	106.340	108.070	109.800	111.520	113.230	114.920	116.590	118.210	119.770	121.200	122.230
16	91.525	91.479	91.337	92.180	92.872	94.335	95.910	97.559	99.258	100.990	102.740	104.490	106.250	108.010	109.750	111.490	113.210	114.910	116.580	118.210	119.770	121.200	122.230
15	91.526	91.482	91.348	92.238	93.036	93.732	95.427	97.175	98.958	100.760	102.560	104.370	106.160	107.940	109.710	111.460	113.190	114.900	116.570	118.200	119.770	121.200	122.240
14	91.540	91.498	91.372	92.339	93.245	94.090	94.887	96.752	98.638	100.520	102.390	104.250	106.080	107.890	109.670	111.440	113.180	114.890	116.570	118.210	119.780	121.210	122.240
13	91.562	91.522	91.402	92.454	93.466	94.438	95.383	96.310	98.325	100.310	102.250	104.150	106.020	107.850	109.650	111.430	113.180	114.900	116.580	118.220	119.790	121.220	122.260
12	91.587	91.549	91.433	92.571	93.680	94.766	95.843	96.928	98.057	100.140	102.150	104.090	105.990	107.840	109.660	111.440	113.200	114.920	116.610	118.250	119.820	121.250	122.280
11	91.614	91.576	91.463	92.680	93.877	95.062	96.249	97.456	98.714	100.060	102.120	104.100	106.020	107.880	109.700	111.480	113.230	114.960	116.640	118.280	119.850	121.280	122.320
10	91.639	91.602	91.491	92.779	94.052	95.321	96.596	97.896	99.244	100.670	102.190	104.180	106.100	107.960	109.770	111.540	113.290	115.010	116.690	118.320	119.890	121.320	122.360
9	91.662	91.625	91.515	92.865	94.203	95.540	96.887	98.257	99.669	101.140	102.690	104.340	106.250	108.080	109.870	111.630	113.360	115.070	116.740	118.380	119.940	121.370	122.400
8	91.683	91.646	91.536	92.938	94.330	95.723	97.125	98.549	100.010	101.520	103.090	104.740	106.480	108.240	109.990	111.730	113.450	115.140	116.810	118.430	119.990	121.420	122.450
7	91.700	91.663	91.553	92.998	94.435	95.872	97.318	98.782	100.270	101.810	103.380	105.020	106.700	108.410	110.130	111.840	113.540	115.220	116.880	118.490	120.050	121.470	122.510
6	91.714	91.677	91.567	93.046	94.519	95.991	97.470	98.964	100.480	102.030	103.610	105.230	106.890	108.560	110.250	111.940	113.620	115.290	116.940	118.550	120.100	121.520	122.560
5	91.725	91.689	91.578	93.084	94.584	96.083	97.587	99.104	100.640	102.200	103.780	105.390	107.030	108.690	110.360	112.030	113.700	115.360	117.000	118.610	120.150	121.570	122.600
4	91.734	91.697	91.586	93.112	94.632	96.151	97.674	99.207	100.750	102.320	103.910	105.520	107.140	108.790	110.450	112.110	113.770	115.420	117.050	118.650	120.190	121.610	122.640
3	91.740	91.703	91.592	93.132	94.666	96.198	97.734	99.277	100.830	102.400	103.990	105.600	107.220	108.860	110.510	112.160	113.810	115.460	117.090	118.690	120.230	121.640	122.670
2	91.744	91.706	91.595	93.144	94.686	96.226	97.769	99.319	100.880	102.450	104.040	105.650	107.270	108.900	110.550	112.200	113.840	115.490	117.110	118.710	120.250	121.660	122.690
1	91.745	91.708	91.596	93.147	94.692	96.235	97.780	99.332	100.890	102.470	104.060	105.660	107.280	108.920	110.560	112.210	113.850	115.500	117.120	118.720	120.250	121.670	122.700

VKD Kx and Ky (m/day) by row and column

(VKDGrad = 0.6 * Kx)

	1	2	3	4	5	6	7	8	9	10	11
21	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
20	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
19	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
18	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
17	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
16	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
15	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
14	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
13	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
12	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
11	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
10	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
9	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
8	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
7	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
6	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
5	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
4	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
3	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
2	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096
1	21.579	21.579	21.579	21.483	21.369	21.233	21.073	20.884	20.663	20.402	20.096

12	13	14	15	16	17	18	19	20	21	22	23
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857
19.736	19.310	18.805	18.201	17.475	16.592	15.507	14.151	12.425	10.173	7.137	2.857

Leakage node parameters

X (m)	Y (m)	Elevation (m)	Conductance (day^{-1})
1000	0	101	0.02
1000	500	101	0.02
1000	1000	101	0.02
1000	1500	101	0.02
1000	2000	101	0.02
1000	2500	101	0.02
1000	3000	101	0.02
1000	3500	101	0.02
1000	4000	101	0.02
1000	4500	101	0.02
1000	5000	101	0.02
1000	5500	101	0.02
1000	6000	101	0.02
1000	6500	101	0.02
1000	7000	101	0.02
1000	7500	101	0.02
1000	8000	101	0.02
1000	8500	101	0.02
1000	9000	101	0.02
1000	9500	101	0.02
1000	10000	101	0.02

River node parameters

X (m)	Y (m)	River Stage (m)
1500	8000	101.75
2000	7500	101.9
2500	7000	102.4
3000	6500	103.3
3500	6000	104.5
4000	5500	106.1
4500	5000	108
5000	4500	110
5500	4000	112
6000	4000	114
6500	4000	116
7000	4000	118
7500	4000	120.4
8000	4000	122.8
8500	3500	125.2
9000	3000	127.6
9500	2500	130

Bed Elevation (m)	Length (m)	Width (m)	Bed Conductance (day^{-1})	Bed Thickness (m)
101.75	1	1	3000	0.5
101.9	1	1	3000	0.5
102.4	1	1	3000	0.5
103.3	1	1	3000	0.5
104.5	1	1	3000	0.5
106.1	1	1	3000	0.5
108	1	1	3000	0.5
110	1	1	3000	0.5
112	1	1	3000	0.5
114	1	1	2700	0.5
116	1	1	2400	0.5
118	1	1	2100	0.5
120.4	1	1	1800	0.5
122.8	1	1	1500	0.5
125.2	1	1	1200	0.5
127.6	1	1	900	0.5
130	1	1	600	0.5

Initial water table elevation (m) for Test 2 and 3 models

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
21	101.6174	101.5855	101.4903	102.5551	103.6432	104.7765	105.9647	107.2082	108.5025	109.8405	111.2140	112.6151	114.0361	115.4703	116.9113	118.3530	119.7894	121.2133	122.6156	123.9817	125.2847	126.4586	127.2419
20	101.6111	101.5788	101.4831	102.5308	103.6082	104.7375	105.9263	107.1731	108.4720	109.8149	111.1930	112.5983	114.0229	115.4601	116.9035	118.3472	119.7850	121.2101	122.6133	123.9800	125.2835	126.4576	127.2410
19	101.5930	101.5591	101.4601	102.4508	103.4963	104.6157	105.8086	107.0671	108.3806	109.7386	111.1310	112.5488	113.9842	115.4302	116.8808	118.3302	119.7725	121.2010	122.6067	123.9753	125.2800	126.4549	127.2384
18	101.5661	101.5281	101.4170	102.2880	103.2842	104.3968	105.6048	106.8878	108.2288	109.6136	111.0304	112.4695	113.9227	115.3833	116.8455	118.3041	119.7535	121.1874	122.5971	123.9686	125.2752	126.4513	127.2351
17	101.5387	101.4939	101.3537	101.9675	102.9278	104.0595	105.3063	106.6339	108.0190	109.4443	110.8965	112.3654	113.8432	115.3235	116.8014	118.2720	119.7307	121.1715	122.5863	123.9615	125.2706	126.4481	127.2324
16	101.5246	101.4785	101.3373	101.9297	102.3721	103.5852	104.9101	106.3090	107.7579	109.2386	110.7374	112.2444	113.7527	115.2570	116.7534	118.2382	119.7075	121.1563	122.5768	123.9561	125.2680	126.4470	127.2318
15	101.5262	101.4818	101.3479	101.9882	102.5364	102.9822	104.4275	105.9248	107.4579	109.0089	110.5647	112.1170	113.6603	115.1914	116.7080	118.2078	119.6882	121.1450	122.5714	123.9548	125.2693	126.4499	127.2351
14	101.5402	101.4981	101.3721	102.0888	102.7455	103.3400	103.8869	105.5016	107.1383	108.7734	110.3947	111.9967	113.5772	115.1358	116.6723	118.1865	119.6772	121.1414	122.5729	123.9598	125.2766	126.4585	127.2440
13	101.5619	101.5218	101.4020	102.2044	102.9657	103.6885	104.3829	105.0603	106.8249	108.5561	110.2475	111.8999	113.5163	115.1000	116.6540	118.1801	119.6790	121.1486	122.5838	123.9732	125.2915	126.4743	127.2601
12	101.5874	101.5488	101.4333	102.3208	103.1797	104.0163	104.8426	105.6781	106.5573	108.3894	110.1475	111.8449	113.4912	115.0942	116.6602	118.1937	119.6970	121.1694	122.6062	123.9964	125.3153	126.4984	127.2842
11	101.6138	101.5761	101.4633	102.4304	103.3771	104.3122	105.2487	106.2062	107.2141	108.3137	110.1211	111.8499	113.5150	115.1272	116.6967	118.2310	119.7338	121.2052	122.6409	124.0302	125.3483	126.5309	127.3166
10	101.6391	101.6020	101.4908	102.5290	103.5524	104.5705	105.5961	106.6463	107.7439	108.9162	110.1894	111.9299	113.5985	115.2051	116.7667	118.2933	119.7897	121.2559	122.6877	124.0740	125.3901	126.5714	127.3568
9	101.6622	101.6254	101.5151	102.6148	103.7035	104.7902	105.8866	107.0072	108.1693	109.3922	110.6949	112.0938	113.7506	115.3300	116.8687	118.3784	119.8624	121.3195	122.7446	124.1262	125.4391	126.6185	127.4033
8	101.6825	101.6458	101.5358	102.6876	103.8304	104.9730	106.1253	107.2991	108.5079	109.7657	111.0867	112.4857	113.9850	115.4947	116.9948	118.4799	119.9470	121.3921	122.8087	124.1842	125.4929	126.6700	127.4541
7	101.6998	101.6631	101.5530	102.7477	103.9348	105.1219	106.3178	107.5319	108.7744	110.0555	111.3841	112.7668	114.2029	115.6623	117.1270	118.5871	120.0363	121.4685	122.8757	124.2445	125.5487	126.7231	127.5065
6	101.7141	101.6773	101.5670	102.7962	104.0185	105.2407	106.4701	107.7144	108.9814	110.2782	111.6105	112.9809	114.3862	115.8136	117.2513	118.6902	120.1232	121.5432	122.9412	124.3033	125.6030	126.7747	127.5574
5	101.7254	101.6886	101.5780	102.8342	104.0837	105.3328	106.5874	107.8541	109.1387	110.4466	111.7815	113.1444	114.5330	115.9405	117.3592	118.7818	120.2014	121.6109	123.0008	124.3571	125.6526	126.8219	127.6039
4	101.7340	101.6971	101.5862	102.8625	104.1323	105.4011	106.6742	107.9569	109.2542	110.5699	111.9068	113.2657	114.6447	116.0399	117.4458	118.8567	120.2664	121.6676	123.0510	124.4024	125.6946	126.8618	127.6432
3	101.7400	101.7030	101.5919	102.8821	104.1659	105.4482	106.7338	108.0274	109.3331	110.6541	111.9927	113.3494	114.7231	116.1109	117.5089	118.9120	120.3147	121.7101	123.0889	124.4367	125.7263	126.8920	127.6730
2	101.7435	101.7065	101.5953	102.8935	104.1855	105.4757	106.7686	108.0685	109.3790	110.7032	112.0429	113.3986	114.7696	116.1535	117.5471	118.9458	120.3445	121.7364	123.1124	124.4580	125.7461	126.9109	127.6916
1	101.7447	101.7076	101.5964	102.8973	104.1920	105.4848	106.7801	108.0820	109.3942	110.7193	112.0594	113.4148	114.7850	116.1677	117.5598	118.9572	120.3546	121.7454	123.1204	124.4653	125.7529	126.9173	127.6979

Appendix 2 Test 4 and 5 model ZOOMQ3D VKD files

File Name	File Contents
vkd.dat	vkdkx vkdky vkdgrad vkdztop
vkd.cod	1 1 1 1 (For Test 4 model) 1 1 1 2 (For Test 5 model)
vkd.map **vkdkx01.map** **vkdky01.map** **vkdztop01.map** **vkdgrad01.map**	---- Map for grid on level: 1 SW: 0,0 NE: 11000,10000 ---- aaaaaaaaaaa aaaaaaaaaaa aaaaaaaaaaa aaaaaaaaaaa aaaaaaaaaaa aaaaaaaaaaa aaaaaaaaaaa aaaaaaaaaaa aaaaaaaaaaa aaaaaaaaaaa aaaaaaaaaaa ---- Map for grid on level: 2 SW: 3000,3000 NE: 7000,7000 ---- aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa aaaaaaaaaaaaaaaaaaaaa
vkdkx01.cod **vkdky01.cod**	---- Code data for grid on level: 1 SW: 0,0 NE: 10000,10000 ---- 10.0 1 1.0 ---- Code data for grid on level: 2 SW: 3000,3000 NE: 7000,7000 ---- 10.0 1 1.0
vkdztop01.cod	---- Code data for grid on level: 1 SW: 0,0 NE: 10000,10000 ---- 150.0 1 1.0 ---- Code data for grid on level: 2 SW: 3000,3000 NE: 7000,7000 ---- 150.0 1 1.0
vkdgrad01.cod	---- Code data for grid on level: 1 SW: 0,0 NE: 10000,10000 ---- 0.5 1 1.0 ---- Code data for grid on level: 2 SW: 3000,3000 NE: 7000,7000 ---- 0.5 1 1.0

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