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Enhancements to Modflow-User Guide for Modflow VKD—A modified version of modflow 96 to include variations in hydraulic properties with depth

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

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ENHANCEMENTS TO MODFLOW

USER GUIDE FOR MODFLOW-VKD – A MODIFIED VERSION OF MODFLOW-96 TO INCLUDE VARIATIONS IN HYDRAULIC PROPERTIES WITH DEPTH

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GLOSSARY OF TERMS AND ABBREVIATIONS

Symbol	Description	Variable name in MODFLOW	Dimensions
BAS	Basic	Package: BAS	-
BCF	Block Centred Flow	Package: BCF	-
B _u	Thickness of upper part of VKD layer	VMID (first simulation when auto-conversion is active)	L
CV, CR, CC	Conductance terms	CV, CR, CC	L ² T ⁻¹
E _{Bot}	Elevation of the base of the model layer	BOT	L
E _{Kmax}	Elevation where the hydraulic conductivity reaches its maximum value	EKMAX	L
E _{Mid}	Elevation of the change from constant to varying hydraulic conductivity (point of inflection)	VMID	L
E _{Top}	Elevation of the top of the model layer	TOP	L
f	Hydraulic conductivity gradient factor	VKGRAD	L ⁻¹
F _s	Storage gradient factor	VSGRAD	L ⁻¹
H	Groundwater head	HNEW (current head) HOLD (head in last time step)	L
HCOF	Head coefficient – contains terms for head dependant boundaries	HCOF	L ² T ⁻¹
i, j, k	Row, column and layer numbers	I, J, K	-
K	Hydraulic conductivity	HY	LT ⁻¹
K _{base}	Hydraulic conductivity of the lower part of a VKD layer in MODFLOW-VKD	HY (same as normal hydraulic conductivity)	LT ⁻¹
K _{max}	Maximum hydraulic conductivity factor	VKMAX	-
LAYCON	Layer-type code	LAYCON	-

Symbol	Description	Variable name in MODFLOW	Dimensions
RHS	“Right hand side” – contains terms for sources/sinks and head dependant boundaries	RHS	L^3T^{-1}
S	Storage coefficient	SC1 or SC2	-
S_{base}	Storage coefficient of the lower part of a VSD layer	SC2 (or SC1 depending on value of LAYCON)	-
S_{max}	Maximum storage factor	VSMAX	-
S_s	Specific storage	(becomes SC1 when integrated over saturated thickness)	L^{-1}
Sy	Specific yield	SC2 (or SC1 depending on value of LAYCON)	-
t	Time	TOTIM	T
T	Transmissivity	- (converted to conductance and stored in CC and CR)	L^2T^{-1}
VKD	Variable hydraulic conductivity with depth	-	-
VSD	Variable storage with depth	-	-
W	Source/sink term (flow per unit volume)	(stored in RHS and HCOF)	T^{-1}
x, y, z	Cartesian co-ordinates	-	L
Δt	Time step length	DELT	T

1 INTRODUCTION

The modified version of the MODFLOW groundwater modelling code described in this user guide is based on the 1996 version of the USGS code: MODFLOW-96 (Harbaugh & McDonald, 1996), which in turn was based on an earlier version of the code: MODFLOW-88 (McDonald & Harbaugh, 1988).

This is a revised version of the User Guide originally issued in March 2002. The revised version includes some minor changes to the MODFLOW VKD code (currently MF-VKD7), the results of some further code testing, and an independent peer review of the code and documentation.

The main focus of the modifications to MODFLOW has been to include a representation of the variation of hydraulic conductivity and storage with depth commonly observed in chalk and limestone aquifers. These modifications provide a way to represent in MODFLOW the behaviour of groundwater in fractured systems, such as chalk and limestone formations. In such systems fissure frequency is high near to the surface thus enhancing hydraulic conductivity, specific yield and the hydraulic connection between the aquifer and surface water. The fracture frequency, and hence conductivity and specific yield, reduce considerably with depth.

Traditionally in the UK, chalk and limestone aquifers have been represented in groundwater models as a thin layer representing only the 'active flow zone', which is usually assumed to be between 30 and 60 m thick, with no variation of hydraulic conductivity with depth. These constant hydraulic conductivity models give rise to a linear variation of transmissivity with depth, which is a poor approximation to the observed transmissivity variation. The limited representation of the conditions in the aquifer means that, in order to represent observed behaviour, the modeller may need to employ unrealistic or contrived values for other model parameters such as storage, river conductance, or temporal distribution of recharge. An additional problem with these types of MODFLOW models is that if a severe drought is being simulated, groundwater heads can fall below the normal active flow zone, resulting in cells becoming 'dry', and distorting the pattern of flow. If a low hydraulic conductivity layer is added below the active flow zone to enable 'wetting' of the layer above, the contrast in hydraulic conductivity between the two layers often results in numerical oscillations as cells change between wet and dry, reducing the likelihood that the model will converge.

The modification to MODFLOW where hydraulic properties are allowed to vary with depth within a single model layer provides a solution to these problems. This gives a non-linear relationship between transmissivity and groundwater level, improving the representation of field conditions. The underlying issues and implications of the changes introduced in MODFLOW are detailed in the Project Report NC/00/23 – *Enhancements to Modflow, variations in hydraulic conductivity and storage with depth* (Environment Agency, 2002).

The modifications to the MODFLOW code are based on a code developed at the University of Birmingham (UK) against which the modified MODFLOW code has been benchmarked (Environment Agency, 1999 & 2001). Other changes to the code have been made to aid comparison with the Birmingham University code, and to include a few useful new options.

The new features introduced in MODFLOW that are described in this User Guide can be grouped into those that relate to the implementation of variable hydraulic properties with depth within a layer (Group I) and others, which increase the flexibility and output options of the code (Group II). These features include:

Group I

- a) Variation of horizontal hydraulic conductivity with depth (VKD).
- b) Variation of storage coefficient with depth (VSD).
- c) Auto-conversion option for converting standard MODFLOW-96 steady state models to include VKD and providing initial conditions for time variant simulations.

Group II

- a) Spatially variable anisotropy (Ruskauff & Kladias).
- b) Inter-nodal transmissivity option to allow greater control of model transmissivities and to allow direct comparison with mesh-centred codes.
- c) Option to allow input of X- and Y-direction transmissivities independently.
- d) Explicit transmissivity calculation option (for comparison with other codes), where transmissivity is updated every time step using heads from the previous time step.
- e) Output of calculated transmissivity values to the listing file.
- f) Allow use of direct access binary output files that can be read directly by Groundwater Vistas (Environmental Simulations Inc, 2001).
- g) Progress monitor for the PCG solver package.
- h) Allow convergence to be forced if the convergence criteria are met during the last inner iteration for a specified number of outer iterations (rather than during the first inner iteration as is usual). This is the same technique used to force convergence of the PCG solver in Groundwater Vistas.
- i) Debugging option for the PCG solver.
- j) Allow a specified discharge, abstraction or tributary inflow at any stream cell.
- k) Correction to the cell-by-cell stream flow output, so that where more than one stream reach is defined in a model cell, only the stream flow from the furthest downstream reach is used to compute the accreted stream flow at that point.

MODFLOW is the 'Modular Three-Dimensional Finite-Difference Ground-Water Flow Model' developed by the United States Geological Survey (McDonald & Harbaugh, 1988, Harbaugh & McDonald, 1996). The model is made up of a number of different modules (or packages) that handle different aspects of groundwater simulations, and a main program that handles the calls to the different routines in each of the modules.

The modifications undertaken for the implementation of variable hydraulic conductivity (VKD) and specific yield (VSD) with depth within a layer required changes to the main program and Block-Centred Flow (BCF) module, which defines the conductance and storage terms of the groundwater flow equations, based on the aquifer properties. This leads to changes or new options in the format of the BCF (and name) files required by MODFLOW. The modifications to the code and input files are described in Sections 2, 6 and 8. Section 8 also provides an introduction to a practical application of the code for modelling groundwater systems where parameters vary with depth.

The stream package, a module used to simulate external influences on the groundwater system due to surface water interactions, was also modified as part of this project. The changes to the stream package are outlined in Section 3.

Once the terms of the finite difference groundwater flow equations have been defined (by the BCF and other packages), a number of different solver modules are available to solve these equations. Some modifications were also made to the output options of one of these solver modules; namely, the Preconditioned Conjugate Gradient 2 (PCG2) module. These changes are documented in Section 4.

The Utilities module was also modified slightly. This module contains routines to read data from input files, and write data to output files. The modifications introduced to the Utilities module are described in Section 5.

Finally, a guide to compiling the code and post processing utilities for VKD MODFLOW are presented in Section 7 and 9, respectively.

Appendices A-E list the computer code of the MODFLOW packages where modifications were introduced.

Appendix F describes further testing for MODFLOW VKD (MF-VKD), which was carried out to ascertain that the VKD modifications do not affect the basic functionality of MODFLOW. A series of tests is presented, where the results generated by the unmodified version of MODFLOW 96 (MF96) and MODFLOW-VKD (MF-VKD) with the VKD function active and inactive, are compared to identify whether and why significant discrepancies emerge. The testing is based on a suite of models developed by the US EPA, the USGS, and two models developed for the Environment Agency, the former aiming at water resource assessment in the Wirral peninsula and the latter at the definition of groundwater protection zones for the Tadcaster brewery boreholes. In the test based on the Tadcaster model, MF96 and MF-VKD are coupled with MODPATH to check whether the two programs produce different particle-tracking results. A variation on one of the original test models used for testing MODFLOW-VKD is also employed to run the USGS optimisation and sensitivity analysis program, UCODE, in combination with MODFLOW-VKD. The purpose of this test is to check whether and how UCODE works with MF-VKD. In two of the tests, the results produced by unmodified MODFLOW and the executable of MF-VKD created with the FORTRAN Compaq compiler were compared to check that the use of a different compiler would not affect the model output. The modifications to the input datasets that are required to run MF-VKD and the results of each test are documented in a series of summary sheets. The implications of coupling MF-VKD with MODPATH to perform particle tracking are also discussed.

Appendix G is an independent peer review of the MODFLOW VKD code by Professor David Lerner, Groundwater Protection and Restoration Group, University of Sheffield.

Appendix H provides a summary of the MODFLOW VKD version history.

2 BLOCK-CENTRED FLOW (BCF) PACKAGE

2.1 Introduction

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

MODFLOW uses a finite difference form of the groundwater flow equation:

$$\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial h}{\partial z} \right) - W = S_s \frac{\partial h}{\partial t}$$

Equation (2.1)

where

K_{xx} , K_{yy} and K_{zz} are values of hydraulic conductivity along the x, y and z coordinate axes, which are assumed to be parallel to the major axes of hydraulic conductivity [LT^{-1}];

h is the potentiometric head [L];

W is a volumetric flux per unit volume and represents sources and/or sinks of water [T^{-1}];

S_s is the specific storage of the porous material [L^{-1}]; and

t is time [T].

The finite difference form of equation (1) used in MODFLOW is (McDonald and Harbaugh, 1988):

$$\begin{aligned} & CV_{i,j,k-\frac{1}{2}} h_{i,j,k-1} + CC_{i-\frac{1}{2},j,k} h_{i-1,j,k} + CR_{i,j-\frac{1}{2},k} h_{i,j-1,k} \\ & + (-CV_{i,j,k-\frac{1}{2}} - CC_{i-\frac{1}{2},j,k} - CR_{i,j-\frac{1}{2},k} - CR_{i,j+\frac{1}{2},k} - CC_{i+\frac{1}{2},j,k} - CV_{i,j,k+\frac{1}{2}} + HCOF_{i,j,k}) h_{i,j,k} \\ & + CR_{i,j+\frac{1}{2},k} h_{i,j+1,k} + CC_{i+\frac{1}{2},j,k} h_{i+1,j,k} + CV_{i,j,k+\frac{1}{2}} h_{i,j,k+1} = RHS_{i,j,k} \end{aligned}$$

Equation (2.2)

The *CV*, *CR* and *CC* coefficients are conductances between nodes, defined as the product of hydraulic conductivity and cross-sectional area of flow divided by the length of the flow path (in this case the distance between the nodes). The *HCOF* and *RHS* coefficients are composed of external source terms and storage terms (constant flows such as abstractions are added to *RHS*, whilst head dependent boundary conditions affect both the *HCOF* and *RHS* coefficients). The *i*, *j* and *k* terms relate to the row, column and layer numbers in the model respectively. Besides calculating the conductances and storage terms, the BCF package calculates flow correction terms that are added to *HCOF* and *RHS* when an underlying aquifer becomes partially unsaturated, effectively reducing the downward flow to a constant limiting value. Other functions of the BCF package include the desaturation (drying), and resaturation (wetting) of cells, and alternative formulations for calculating the conductances between cells.

2.2 Conceptualisation and implementation of new features

The following discussion of the conceptualisation and implementation of the new features included in the BCF package is divided into seven sections: Variation of hydraulic conductivity with depth (VKD), Variation of storage with depth (VSD), Initial conditions, Spatially variable anisotropy, Inter-nodal transmissivity, Explicit transmissivity calculation and Transmissivity output option.

2.2.1 Variation of hydraulic conductivity with depth (VKD)

The traditional MODFLOW layer types (LAYCON = 0 to 3) assume either that transmissivity remains constant, or that the hydraulic conductivity within the aquifer layer is constant, resulting in a linear relationship between groundwater head and transmissivity. For many aquifers hydraulic conductivity is a function of depth, and these formulations are inappropriate; especially for aquifers in fractured rock, such as chalk and limestone, where groundwater flow is primarily through fissures which have been enhanced due to groundwater flow near the water table.

Groundwater systems where hydraulic conductivity varies with depth can be simulated using a model with a number of traditional MODFLOW layers, however, if the water table fluctuates through these layers numerical problems associated with desaturation and resaturation of cells can become a problem.

This version of the BCF package introduces two new layer types to represent aquifers where hydraulic conductivity reduces with depth within the layer. The first of these (LAYCON = 4) can be used to represent unconfined layers only, the second (LAYCON = 5) can be used to represent layers that can convert between confined and unconfined depending on the groundwater head.

Conceptual model for variation of hydraulic conductivity with depth

The conceptual model for variation of hydraulic conductivity with depth is based on a modified version of that employed at the University of Birmingham (Rushton *et al*, 1980, 1982 & 1989) and is shown in Figure 2.1. For the lower part of the aquifer, the hydraulic conductivity takes a constant value, K_{base} . Above a reference level the hydraulic conductivity increases linearly, increasing at a rate of f per unit rise in groundwater head, until a maximum value of hydraulic conductivity is reached, K_{max} . f and K_{max} can either be defined in units of hydraulic conductivity or as a multiple of K_{base} depending on the preference of the user. The transmissivity is simply the integral of the hydraulic conductivity between the base and the water table (or between the base and the top if the layer is confined).

This conceptualisation has been tried and tested in many groundwater models of chalk and limestone aquifers constructed by the University of Birmingham and other industry consultants (Salmon *et al*, 1996).

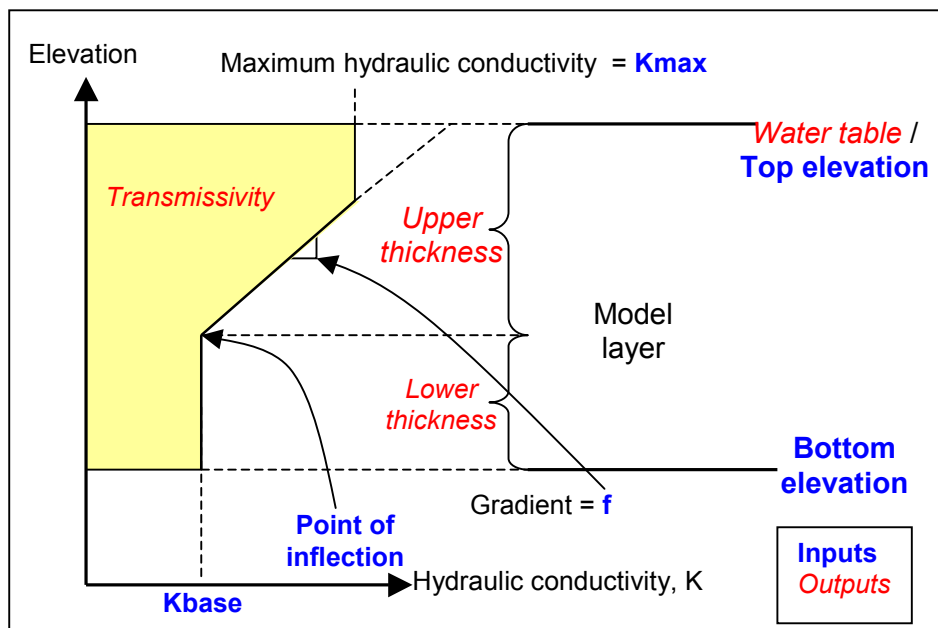


Figure 2.1 Conceptual model for the variation of hydraulic conductivity with depth

Implementation of VKD in MODFLOW

The transmissivity for each cell is calculated each iteration from the following properties:

Base hydraulic conductivity, K_{base} [LT^{-1}]

Bottom elevation, e_{bot} [L]

Elevation of point of inflection, e_{mid} [L]

Hydraulic conductivity gradient (or gradient factor), f [T^{-1}] (or [L^{-1}])

Maximum hydraulic conductivity (or max K factor), K_{max} [LT^{-1}] (or [-])

Top elevation, e_{top} [L]

Groundwater head, h [L]

In the equations below it is assumed that f and K_{max} are in units of hydraulic conductivity rather than as multiples of K_{base} .

The elevation ($e_{K_{max}}$) where the hydraulic conductivity reaches its maximum value is given by

$$e_{k \max} = e_{mid} + \frac{K_{\max} - K_{base}}{f}$$

Equation (2.3)

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

$$T = K_{base} (h - e_{bot})$$

Equation (2.4)

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

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

Equation (2.5)

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

$$T = K_{base} (h - e_{bot}) + \frac{f (e_{K_{max}} - e_{mid})^2}{2} + (K_{max} - K_{base}) (h - e_{K_{max}})$$

Equation (2.6)

If the groundwater head is above the top of the layer (for layer type 5 only) then Equation 2.6 is used with the groundwater head, h , replaced by the top elevation, e_{top} .

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

Notice that Equation 2.5 includes a term with groundwater head (h) squared. Introducing the squared term makes the mathematical problem non-linear. Such problems are inherently harder to solve. In this case the transmissivity (and hence the conductance terms) can change dramatically as the groundwater head values are updated at each node during each iteration of the solver routines. This can have a detrimental effect on simulation convergence.

Issues relating to convergence

As a result of the non-linear relationship between groundwater head and transmissivity, simulations using VKD can be subject to instabilities. This is due to groundwater head values being over or underestimated as the transmissivity values are updated each iteration. This is especially true for steady-state simulations, where the initial conditions need to be close enough to the actual solution in order for the simulation to converge. The automatic conversion option (for converting standard MODFLOW-96 models to VKD models – see Section 2.2.3) has been developed to avoid these instability problems.

Whilst VKD produces a non-linear relationship between groundwater head and transmissivity, it also causes a reduction in the variation of groundwater heads (when heads are above the point of inflection) compared to simulations that use an average hydraulic conductivity. This reduction in head variations means that, when running time-variant simulations, the heads from the last time step are likely to be closer to the solution for the current time step, therefore requiring fewer iterations to converge. This coupled with the general damping effect of aquifer storage, means that time-variant VKD simulations are far more stable than steady-state VKD simulations.

If problems are experienced with time variant simulations, an option has been added that enables the code to use the groundwater head from the last time step in the transmissivity calculations (set IHOLD to 1 – see Section 2.2.6). This means that the transmissivity is held constant throughout a time step, which may improve convergence in time-variant simulations. This explicit formulation for the transmissivity calculations is not as accurate as the implicit formulation (default), and may even result in reduced stability if large time steps are used.

2.2.2 Variation of storage with depth (VSD)

Associated with the reductions in horizontal hydraulic conductivity, there is also evidence of reductions in storage with depth in fissured groundwater systems (Owen and Robinson, 1978, Southern Water Authority, 1979). Therefore, to complement the variation of hydraulic conductivity with depth, the new layer types in MODFLOW (LAYCON = 4 or 5) also allow variations in storage coefficient (specific yield) with depth (VSD). It should be noted that this feature can cause instabilities and problems with convergence and it is recommended that its use be avoided unless the field evidence suggests that it is an important feature of the catchment.

Conceptual model for S variation with depth

The conceptual model for variation of storage with depth is based on that for the variation of hydraulic conductivity with depth and is shown in Figure 2.2. For the lower part of the aquifer, the specific yield takes a constant value, S_{base} . Above a reference level (independent of that for hydraulic conductivity) the storage increases linearly, increasing at a rate of F_S per unit rise in groundwater head, until a maximum value of storage is reached, S_{max} . F_S and S_{max} can either be defined in units of specific yield or as a multiple of S_{base} depending on the preference of the user. The storage accessible from the aquifer depends on the level of the water table within this profile.

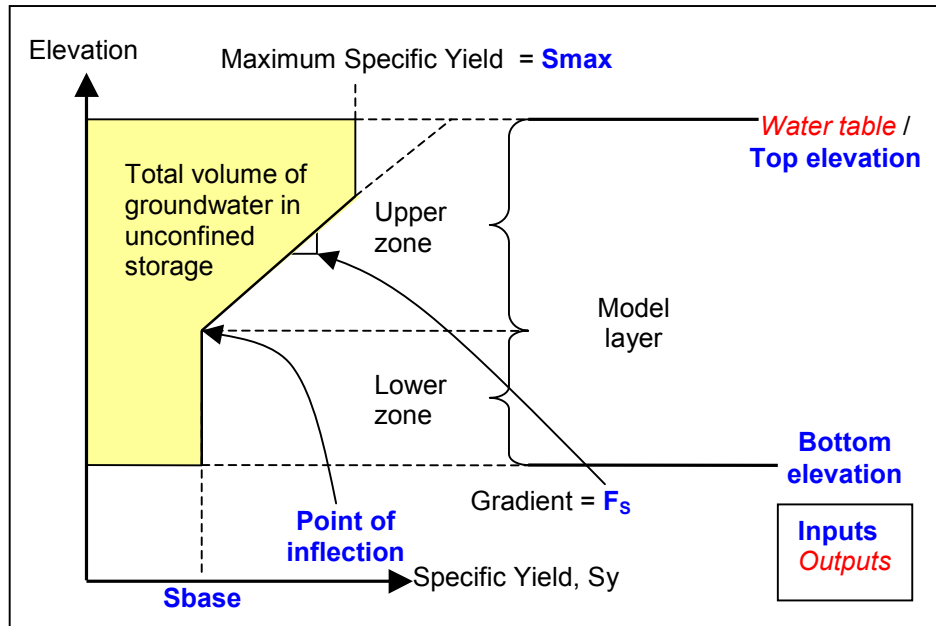


Figure 2.2 Conceptual model for the variation of storage with depth

A problem related to the use of VSD when both confined and unconfined storage coefficients are employed was discovered and corrected in January 2003. The problem emerged whenever the point of inflection of the VSD profile was set above the top elevation of the model layer, and consisted in not replacing specific yield with the confined storage coefficient when calculating flows to and from storage.

Implementation of VSD

The part of the groundwater flow equation (2.1) that relates to the flows to and from storage is the last term in Equation 2.1:

$$S \frac{\partial h}{\partial t}$$

Equation (2.7)

when S is constant, the finite difference form of this term can be written as:

$$S(h-h^*)/\Delta t$$

Equation (2.8)

Where S is the storage coefficient,
 h is the head in the current time step,
 h^* is the head from the previous time step, and
 Δt is the time step length.

This can be substituted into the constant flux (RHS) and head dependent ($HCOF$) terms of equation 2.2 as:

$$\begin{aligned} RHS &= -S h^*/\Delta t \\ HCOF &= -S/\Delta t \end{aligned}$$

Equation (2.9)

However, when the storage changes as a function of groundwater head (as in Figure 2.3 below), the flows to or from storage can be proportional to the square of the change in groundwater head. As terms relating to the square of groundwater head are not included in Equation 2.2, an approximation has to be made. The approximation assumes that when the solution has converged the change in groundwater head between iterations is small enough that the corresponding change in storage coefficient is negligible.

If the head is in the variable storage zone, the assumption that the change in storage coefficient is negligible is incorrect at the start of a time step. Therefore the storage coefficient used at the start of an iteration is inconsistent with the head at the end, leading to water a balance error. This means that the storage coefficient must be updated before the next iteration. The approximation is stable if the head has moved between two points in the constant S zone (as the storage coefficient at the beginning and end of the iteration will be equal). However, problems of convergence may occur if the head is in the variable storage zone, when the storage coefficient will change between iterations.

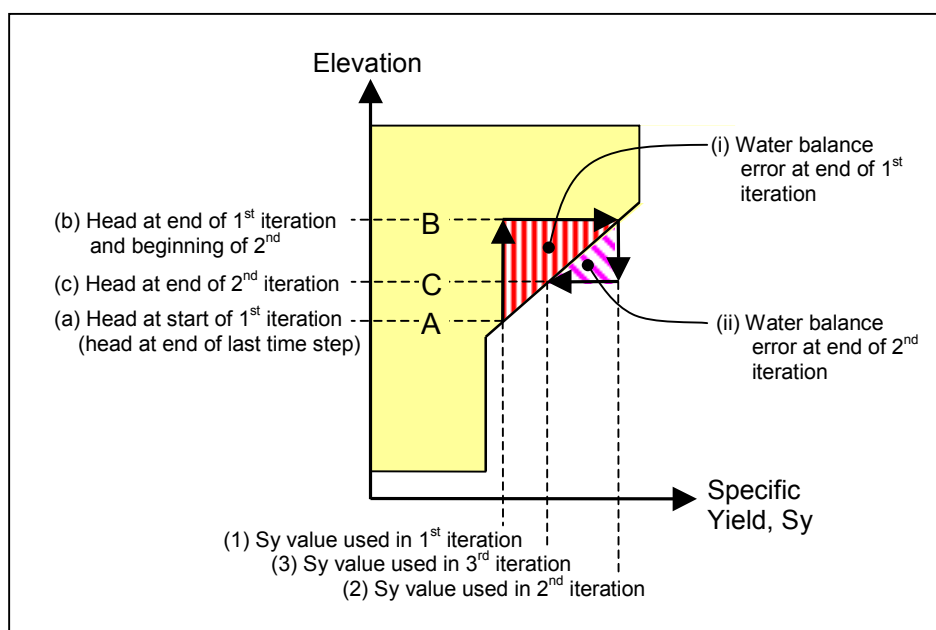


Figure 2.3 Approximation used in VSD calculations

The way the code implements the approximation is to calculate the total water in storage for the head values at the current iteration, and the previous time step (this is shown for the beginning of the 2nd iteration in Figure 2.3 as the shaded area below lines B and A respectively). The total change in storage (the shaded area *between* lines A and B) is then added to the *RHS* coefficient. The *HCOF* coefficient is then given a value reflecting the current storage coefficient (line 2 in Figure 2.3) at the current groundwater head (line B). Finally a correction term equal to the *HCOF* value multiplied by the current groundwater head value is added to the *RHS* coefficient.

This approximation means that the storage coefficient is held constant during each iteration, leading to a water balance error (shown as (ii) in Figure 2.3 for the end of the 2nd iteration). This error should gradually reduce as the changes in head between iterations become smaller. The approximation will converge on a solution once the change in groundwater head between iterations (and hence the change in storage coefficient) is small enough. However large changes in head can often lead to instabilities.

Issues relating to convergence

Problems with non-convergence arise when the storage coefficient changes between iterations. This can also happen when the groundwater head is at the top of the layer, and the storage coefficient changes between confined and unconfined values, but it is most likely to happen when the head is above the point of inflection in the zone of increasing storage. The problem occurs when the groundwater head is calculated using an initial value for the storage coefficient, which then changes based on the new head value. The situation can then arise where the groundwater head fluctuates between levels of different storage coefficient, without converging on a solution.

Simulations that include variations in storage with depth are particularly prone to numerical instabilities due to the approximation in the VSD calculations described above. For this reason it is suggested that this capability should be made inactive (by setting the maximum factor to one) unless the field evidence indicates that it is an important feature of the catchment. However, if the feature is required, a number of methods are available to combat the instabilities and non-convergence. These include:

- Try different combinations of solver parameters. The PCG2 solver is a reliable solver, and is especially good at solving non-linear problems when the maximum number of inner iterations is set to one, and/or the damping factor is set to a low value (see Section 4).
- Reduce the size of the time steps, which reduces the change in heads between time steps and hence minimises the effect of the approximation.
- Minimise the zone of increasing storage by setting the storage gradient, F_s , to a higher value than the maximum storage factor, S_{max} (the distance between the point of inflection and the elevation of maximum storage is equal to $(S_{base} - S_{max})/F_s$, or $(1 - S_{max})/F_s$ if gradient and maximum factors are specified as multiples of S_{base}).
- Avoid setting the elevation of the change in storage to the same as that for hydraulic conductivity. Although conceptually these points may be at the same level, a small offset (~1 metre) may help to reduce instabilities.

2.2.3 Initial conditions: auto-conversion for steady state simulations

As mentioned in Section 2.2.1 (*Issues relating to convergence*) the initial conditions for a steady state VKD simulation need to be similar to the solution in order for the model to converge. For this reason a methodology has been developed where an initial solution is found using a simplified model, the VKD parameters are then introduced and a second simulation with VKD active is started using initial heads from the simplified model. This stepwise approach provides a means of building up the complexity of a model, whilst avoiding numerical instabilities.

Auto-conversion options

As part of the modifications to the MODFLOW code, two new steady state options are available that implement the stepwise approach shown in Figure 2.4 (after page 54). These options can be used to convert a standard MODFLOW-96 model to a model with VKD. The first option converts a model layer with specified transmissivities to a VKD layer, the second option converts a layer with specified hydraulic conductivity to VKD. The following steps are implemented when either of the two new options are activated:

- 1) Depending on the option chosen, model layers in which VKD is required can be assigned either transmissivity or (vertically averaged) hydraulic conductivity values, which are then used in the first simulation to calculate the initial heads. In addition to the transmissivity or hydraulic conductivity values, the user must specify parameters relating to the variation of hydraulic conductivity with depth. These are (see Figure 2.5 and Table 2.1): the upper thickness, the K gradient factor (f), the maximum K factor (Kmax) and the bottom elevation (and top elevation if the layer can become confined). The upper thickness, gradient and maximum factors are not used in the first simulation. When using the auto conversion option the hydraulic conductivity gradient and maximum hydraulic conductivity must be entered in terms of a multiple of the base hydraulic conductivity (absolute values in hydraulic conductivity units are not supported).

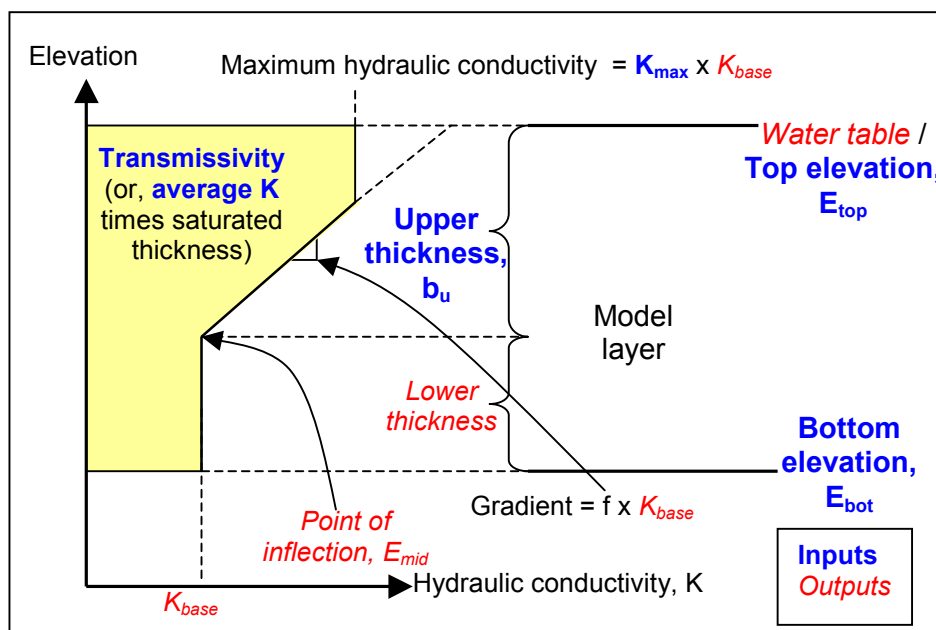


Figure 2.5 Inputs and outputs for automatic conversion option

- 2) Once the first simulation has produced a solution, the parameters required for the VKD simulation (Figure 2.1) are calculated. The elevation of the change in hydraulic conductivity (point of inflection) is calculated from the upper thickness and the calculated head (or top elevation if the node is confined). If the specified upper thickness is greater than the total saturated thickness then it is reduced and messages are written to the output file (the standard MODFLOW listing file for the first simulation). The base hydraulic conductivity (K_{base}) is calculated from the following relationship:

$$K_{base} = \frac{T}{\left(h - E_{bot} - \frac{1}{2f} (K_{max} - 1)^2 + b_u (K_{max} - 1) \right)}$$

Equation (2.10)

If K_{max} is greater than $b_u \times f + 1$, it is higher than the highest possible K attainable by letting K increase linearly up to the water table/ top elevation, as shown in Figure 2.6. In this case K_{base} is calculated as:

$$K_{base} = \frac{T}{\left(h - E_{bot} + \frac{b_u^2 f}{2} \right)}$$

Equation (2.11)

where K_{base} is the base hydraulic conductivity [LT^{-1}],
 T is the transmissivity [L^2T^{-1}],
 h is the groundwater head [L],
 E_{bot} is the elevation of the base of the layer [L],
 f is the hydraulic conductivity gradient factor [L^{-1}] (can not be [T^{-1}]),
 K_{max} is the maximum hydraulic conductivity factor [-] (can not be [LT^{-1}]), and
 b_u is the thickness of the upper part of the layer [L].

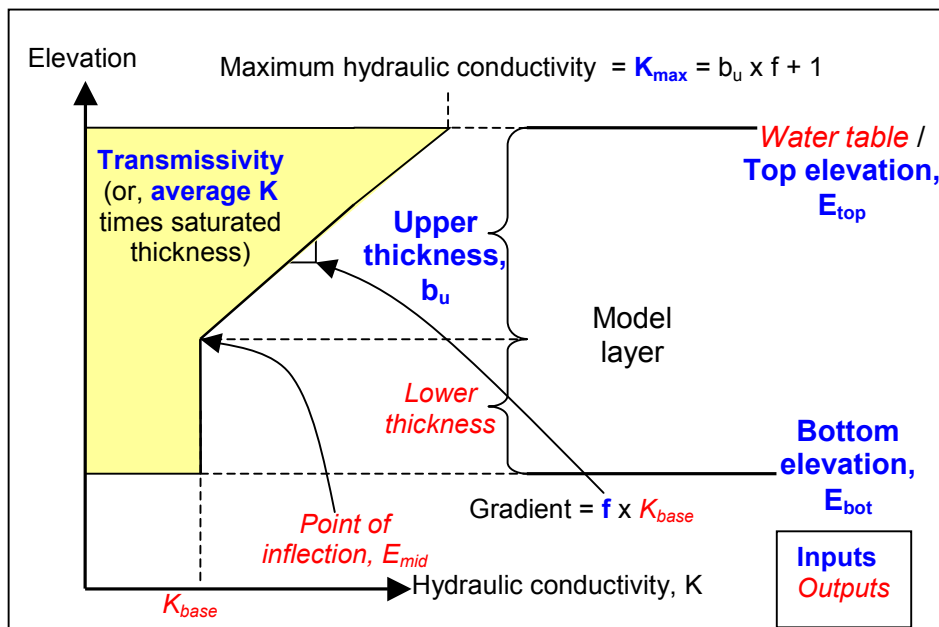


Figure 2.6 Hydraulic conductivity profile when K_{max} is greater than $b_u \times f + 1$

The calculated values are then written to a new BCF file, the initial heads are written to a new BAS (basic) file, and a new NAME file is created with references to both these new files, any other input files from the original model, and new output files.

The formats for the arrays in the new BCF and BAS files remain as they were in the original files, with the exception of the newly calculated variables (initial heads, base hydraulic conductivity and point of inflection) which are automatically given formats with a high degree of precision (10E23.16). The hydraulic conductivity gradient and maximum factors are written in terms of multiples of the base hydraulic conductivity (IKBASE is zero).

The names of the new BAS, BCF and output files can be specified in the original NAME file (see Section 6.2). If output file names are omitted, the original filenames are used with the last character of the filename replaced with a "2" (eg, "Run1.ba2", "Run1.bc2", "Run1.hd2", etc). The new NAME file is always given the same name as the original NAME file, with the last character replaced with a "2" (eg, "Run1.na2").

- 3) The second simulation is then started automatically using the new input files. The results of the second simulation should be virtually identical to those from the first simulation. This can be verified by checking that the drawdowns from the second simulation are very close to zero (the drawdowns should be less than twice the head convergence criteria, and any differences in flow should be less than twice the flow convergence criteria).

Table 2.1 Inputs and outputs for the first simulation of an auto-conversion run

Symbol	Inputs for first simulation		Dimensions
	Description	Variable name in MODFLOW	
T (or K)	Transmissivity (or hydraulic conductivity)	Tran (stored in CC array) (or HY)	L^2T^{-1} (or LT^{-1})
E_{bot}	Bottom elevation	BOT	L
E_{top}	Top elevation (for LAYCON = 5 only)	TOP	L
f	Hydraulic conductivity gradient (or gradient <i>factor</i>)	VKGRAD	T^{-1} (or L^{-1})
K_{max}	Maximum hydraulic conductivity (or max K <i>factor</i>)	VKMAX	LT^{-1} or -
b_u	Upper thickness	VMID	L
H	Groundwater head (water table if unconfined)	HNEW	L
K_{base}	Base hydraulic conductivity	HY	LT^{-1}
E_{mid}	Point of inflection	VMID	L
-	Lower thickness	-	L

For a more detailed description of the inputs required for each of the options see the input instructions (Section 2.3).

2.2.4 *Spatially variable anisotropy (X- & Y-direction transmissivities)*

These code changes are based on those described by Ruskauff and Kladias (1996) and were the first to be implemented as an introduction to modifying the code and to allow comparison with the Birmingham University code (against which the modified MODFLOW code was tested). MODFLOW-96 allows column to row anisotropy to vary only between different layers. Some geologic settings may require a variable anisotropic formulation within a layer in order to be properly represented. For instance, fracturing may be more pronounced along the crest of an anticline than the flanks, dissolution of limestone more intense near discharge areas, and channel deposits abutting overbank deposits.

Modifications to the code were made to allow each grid block in the model to have its own anisotropy, and still retain backward compatibility with the original formulation. Further modifications were then made to allow X- and Y-direction transmissivities or hydraulic conductivities to be specified directly.

2.2.5 *Internodal transmissivity/hydraulic conductivity*

This change to the code was made primarily to allow a direct comparison with the Birmingham University VKD modelling code (which is node-centred rather than block-centred like MODFLOW). However, it does have the added advantage of giving greater control over a model's transmissivity distribution, especially when used in conjunction with the variable anisotropy option.

MODFLOW-96 calculates the conductance between a pair of model nodes based on an average of the transmissivities specified (or calculated) for those nodes. A number of different averaging techniques are available, including harmonic, arithmetic, or logarithmic means. However, all these techniques produce conductances derived from the properties assigned to both the cells. This modification allows inter-nodal transmissivities (or hydraulic conductivities) to be specified for a model layer. In this case each nodes transmissivity value is applied between that node and the next node to the right (for transmissivity along rows) or between the node and the next node to the front (for transmissivity along columns). For unconfined aquifers, the arithmetic mean of the groundwater heads (and bottom elevations and other properties) is used to calculate the conductances. This modification also allows MODFLOW to be compared with node-centred codes such as the Birmingham University code, (provided that parameter values (ie, recharge, storage, transmissivity, etc) are halved at edge nodes, and quartered at corner nodes). It also allows greater control of the parameter values used in the flow equations, especially for modelling narrow features associated with rivers or faults.

2.2.6 *Explicit transmissivity calculation*

Another change that was required to allow a direct comparison with the Birmingham University code was to include an option that keeps calculated transmissivities constant during a time step. If this option is selected then the heads from the previous time step are used to calculate the transmissivity, rather than the heads from the previous iteration. This formulation is slightly less accurate than the implicit formulation used as default, but has the advantage of reducing the number of iterations required for convergence. However, it should be noted that although this option does not make the formulation of the finite difference equations fully explicit, it is still possible that oscillations may be produced in the time-variant solution if there are large changes in head between time steps.

2.2.7 Transmissivity output option

This option has been included to enable the results of the transmissivity calculations to be checked. If the option is selected, the calculated X- and Y-direction inter-nodal transmissivities are written to either the output file (the text-formatted listing file), or a binary output file at the end of each time step. The values can then be checked using a text editor. It is not recommended that this option be used for time-variant models, as the output files produced can be very large.

2.3 Input instructions

2.3.1 Summary of new options

This new version of the MODFLOW modelling code allows a number of new options to be set (shown in bold) in the input instructions for the BCF package. A summary of the inputs required for a VKD simulation is provided in Table 2.2 (Section 2.3.4). The new code should still be compatible with old MODFLOW input files (versions up to MODFLOW-96). The new options included are:

- **Spatially variable anisotropy** - set **ITRPY = 1** and use an array for TRPY for each layer
- **X & Y-direction transmissivities or hydraulic conductivities** - set **ITRPY = 2** and include a 2nd array following the original transmissivity or hydraulic conductivity arrays
- **Explicit transmissivity calculation (more stable)** - set **IHOLD = 1**
- **Write calculated transmissivity values to the listing file** - set **ITRANS <> 0** (not recommended for transient simulations)
- **Internodal transmissivity / hydraulic conductivity** - set **LAYAVG = 40** (first digit of LAYCON = 4X)
- **Variable hydraulic conductivity (VKD) and specific yield with depth (VSD) – unconfined** - set **LAYCON = 4** (last digit of LAYCON = X4) and include the **VMID, VKGRAD & VKMAX** arrays (also **VSMID, VSGRAD & VSMAX** arrays if time variant)
- **Variable hydraulic conductivity (VKD) and specific yield with depth (VSD) – confined / unconfined** - set **LAYCON = 5** (last digit of LAYCON = X5) and include the **TOP, VMID, VKGRAD & VKMAX** arrays (also **VSMID, VSGRAD & VSMAX** arrays if time variant)
- **Alternative steady state options for VKD simulations** - Set **ISS = 2** (Converts specified transmissivity layers to VKD layers) or set **ISS = 3** (Converts specified hydraulic conductivity layers to VKD layers). Layers to be converted should be specified as **LAYCON = X4** or **X5** (other layer types will not be affected) and include the **BOT, Upper Thickness, VKGRAD & VKMAX** arrays

2.3.2 Input format

As this version of the code is based on MODFLOW-96, free-format input is permitted (note: if an old free-format input file does not work, four zeros may need to be added to the end of the first line of the BCF file for ITRPY, IHOLD, ITRANS and IKBASE). The following shows the input instructions for the new BCF package (including format codes for fixed format input, and modules used to read arrays).

Read in subroutine BCF5AL

1. Data: ISS IBCFCB HDRY IWDFLG WETFCT IWETIT IHDWET ITRPY IHOLD ITRANS IKBASE
Format: I10 I10 F10.0 I10 F10.0 I10 I10 I10 I10 I10 I10
2. Data: LAYCON(NLAY) (Maximum of 200 layers)
Format: 40I2

(If there are 40 or fewer layers, use one record; otherwise, use two or more records, with 40 values in each record.)

Read in subroutine BCF5RP

IF ANISOTROPY IS SPECIFIED FOR EACH LAYER (**ITRPY = 0**)

3. Data: TRPY(NLAY)
Module: U1DREL

IF ANISOTROPY IS SPECIFIED FOR EACH NODE (ITRPY is not 0 or 2)

- 3a. Data: TRPY(NCOL,NROW,NLAY)
Module: U2DREL

:
(Repeat for each layer.)

REQUIRED FOR ALL SIMULATIONS

4. Data: DELR(NCOL)
Module: U1DREL
5. Data: DELC(NROW)
Module: U1DREL

A subset of the following two-dimensional arrays is used to describe each layer. The arrays needed for each layer depend on the layer-type code (LAYCON), whether the simulation is transient (ISS=0) or steady state (ISS not 0), if the wetting capability is active (IWDFLG not 0), and whether nodal anisotropy values are used (ITRPY not 0). If an array is not needed, it must be omitted. In no situation will all arrays be required. The required arrays (items 6-19) for layer 1 are read first; then the arrays for layer 2, etc.

IF THE SIMULATION IS TRANSIENT (ISS = 0)

6. Data: Sf1(NCOL,NROW)
Module: U2DREL

IF THE LAYER-TYPE CODE (LAYCON) IS 0 OR 2

7. Data: TranX(NCOL,NROW)
Module: U2DREL

IF THE LAYER-TYPE CODE (LAYCON) IS 0 OR 2, AND TRANSMISSIVITY IS SPECIFIED IN BOTH X- AND Y-DIRECTIONS (ITRPY = 2)

**7a. Data: TranY(NCOL,NROW)
Module: U2DREL**

IF THE LAYER-TYPE CODE (LAYCON) IS 1, 3, 4 OR 5

8. Data: HY(NCOL,NROW)
Module: U2DREL

IF THE LAYER-TYPE CODE (LAYCON) IS 1, 3, 4 OR 5 AND HYDRAULIC CONDUCTIVITY IS SPECIFIED IN BOTH X- AND Y-DIRECTIONS (ITRPY = 2)

**8a. Data: Hy-y(NCOL,NROW)
Module: U2DREL**

IF THE LAYER-TYPE CODE (LAYCON) IS 1, 3, 4 OR 5

9. Data: BOT(NCOL,NROW)
Module: U2DREL

IF NOT THE BOTTOM LAYER

10. Data: Vcont(NCOL,NROW)
Module: U2DREL

IF THE SIMULATION IS TRANSIENT (ISS=0) AND THE LAYER-TYPE CODE (LAYCON) IS 2, 3 OR 5

11. Data: Sf2(NCOL,NROW)
Module: U2DREL

IF THE LAYER-TYPE CODE (LAYCON) IS 2, 3 OR 5

12. Data: TOP(NCOL,NROW)
Module: U2DREL

IF THE LAYER-TYPE CODE (LAYCON) IS 1, 3, 4 OR 5, AND THE WETTING CAPABILITY IS ACTIVE (IWDFLG IS NOT 0)

13. Data: WETDRY(NCOL,NROW)
Module: U2DREL

IF THE LAYER-TYPE CODE (LAYCON) IS 4 OR 5

14. Data: VMID(NCOL,NROW)
Module: U2DREL

IF THE LAYER-TYPE CODE (LAYCON) IS 4 OR 5

15. Data: VKGRAD(NCOL,NROW)
Module: U2DREL

IF THE LAYER-TYPE CODE (LAYCON) IS 4 OR 5

16. Data: VKMAX(NCOL,NROW)
Module: U2DREL

IF THE SIMULATION IS TRANSIENT (ISS=0) AND THE LAYER-TYPE CODE (LAYCON) IS 4 OR 5

17. Data: VSMID(NCOL,NROW)
Module: U2DREL

IF THE SIMULATION IS TRANSIENT (ISS=0) AND THE LAYER-TYPE CODE (LAYCON) IS 4 OR 5

18. Data: VSGRAD(NCOL,NROW)
Module: U2DREL

IF THE SIMULATION IS TRANSIENT (ISS=0) AND THE LAYER-TYPE CODE (LAYCON) IS 4 OR 5

19. Data: VSMAX(NCOL,NROW)
Module: U2DREL

2.3.3 Explanation of parameters used in input instructions

ISS is the steady-state flag

If ISS is not 0, the simulation is steady state.

If ISS = 0, the simulation is transient.

If ISS = 2, two steady state simulations are run. The first simulation uses specified *transmissivities* (input into the HY array) for VKD layers (LAYCON is 4 or 5 – see below), the second uses the variable hydraulic conductivity with depth (VKD) parameters. In this case the original BCF package should have the thickness (not elevation) of the upper zone input into the VMID array. Secondary BCF, BAS and NAM files are created after the first simulation (filenames for these files can be specified in the name file – see Section 6.2). These are used to set up the second simulation.

If ISS = 3, two steady state simulations are run. The first simulation uses specified *hydraulic conductivities* (input into the HY array) for VKD layers (LAYCON is 4 or 5 – see below), the second uses the variable hydraulic conductivity with depth (VKD) parameters. In this case the original BCF package should have the thickness (not elevation) of the upper zone input into the VMID array. Secondary BCF, BAS and NAM files are created after the first simulation (filenames for these files can be specified in the name file – see Section 6.2). These are used to set up the second simulation.

IBCFCB is a flag and a unit number.

If IBCFCB > 0, it is the unit number on which cell-by-cell flow terms will be recorded whenever ICBCFL (see Output Control in McDonald and Harbaugh [1988, p. 4-15]) is set; the terms which are saved will include cell-by-cell storage terms, cell-by-cell constant head flows, and cell-by-cell flow between adjacent cells.

If IBCFCB = 0, cell-by-cell flow terms will not be printed or recorded

If IBCFCB < 0, flow for each constant-head cell will be printed in the listing file whenever ICBCFL is set; cell-by-cell storage terms and cell-by-cell flow between adjacent cells will not be recorded or printed

HDRY is the head that is assigned to cells that are converted to dry during a simulation. Although this value plays no role in the model calculations, it is useful as an indicator when looking at the resulting heads that are output from the model. HDRY is thus similar to HNOFLO in the Basic Package, which is the value assigned to cells that are no-flow cells at the start of a model simulation. It is wise to use a value of HDRY which is below the bottom of the lowest part of the aquifer. This avoids dry cells from becoming active if heads are to be used as starting conditions for a subsequent run

IWDFLG is a flag that determines if the wetting capability is active.

If IWDFLG = 0, the wetting capability is inactive.

If IWDFLG is not 0, the wetting capability is active

WETFCT is a factor that is included in the calculation of the head that is initially established at a cell when it is converted from dry to wet. (see IHDWET).

IWETIT is the iteration interval for attempting to wet cells. Wetting is attempted every IWETIT iterations. If using the PGG solver (Hill, 1990), this applies to outer iterations, not inner iterations. If IWETIT is 0, it is changed to 1.

IHDWET is a flag that determines which equation is used to calculate the initial head at cells that become wet:

If IHDWET = 0, equation (3a) is used:

$$H = BOT + WETFCT (h_n - BOT),$$

(h_n = head in neighbouring cell causing cell to wet)

If IHDWET is not 0, equation (3b) is used:

$$H = BOT + WETFCT (THRESH).$$

ITRPY is a flag that determines whether the anisotropy factor (TRPY) is specified for each layer or for each node

If ITRPY = 0, anisotropy (TRPY) is a one-dimensional array with one value per layer

If ITRPY is not 0 and not 2, anisotropy (TRPY) is a three-dimensional array with a value for each cell

If ITRPY = 2, anisotropy (TRPY) is a three-dimensional array with a value for Y-direction transmissivities or hydraulic conductivities for each cell (X-direction values remain in the TranX or HY array).

IHOLD is a flag that determines whether the calculation of transmissivity (for LAYCON values of 1, 3, 4 or 5) uses the heads calculated in the previous timestep (explicit formulation) or those calculated in the previous iteration (implicit formulation).

If IHOLD = 0, the transmissivity is updated every iteration using the groundwater heads from the current timestep (implicit – slower but more accurate – normal MODFLOW formulation).

If IHOLD = 1, the transmissivity is updated every timestep using the groundwater heads from the previous timestep (explicit – quicker and more stable).

ITRANS is a flag that allows the calculated internodal transmissivities to be output to the listing file every timestep

If **ITRANS = 0**, internodal transmissivity will not be output to the listing file

If **ITRANS > 0**, internodal transmissivity will be output to the listing file every timestep. Not recommended for transient simulations.

If **ITRANS < 0**, it is the unit number on which internodal transmissivity will be recorded whenever **IHDDFL** (see **Output Control** in McDonald and Harbaugh [1988, p. 4-15]) is set. The values are written to a binary file using the same format as the head and drawdown output files. The file must be specified in the name file (Section 6.2)

IKBASE is a flag that denotes whether **VKGRAD** and **VKMAX** will be defined as a multiple of **HY** per unit length or in units of hydraulic conductivity per unit length (and whether **VSGRAD** and **VSMAX** will be defined as a multiple of **Sf** per unit length or in units of specific yield per unit length)

If **IKBASE = 0**, **VKGRAD** and **VKMAX** will be entered as multiples of **HY** per unit length. **VSGRAD** and **VSMAX** will be entered as multiples of **Sf1** or **Sf2** per unit length (depending which represents specific yield – denoted by the value of **LAYCON**)

If **IKBASE** is not 0, **VKGRAD** and **VKMAX** will be entered in units of hydraulic conductivity per unit length. **VSGRAD** and **VSMAX** will be entered in units of specific yield per unit length

LAYCON is the layer-type code consisting of two parts. The first digit (multiplied by 10) gives the averaging method to be used for calculation of the branch conductances (**LAYAVG**). The second digit describes the layer type (**LAYCON**). Each element holds the code for the respective layer. Read both values for each layer. There is a limit of 200 layers. If there are 40 or fewer layers, use one record; otherwise, use two or more records. Leave unused elements in a record blank

LAYAVG:

00 – Harmonic averaging of nodal transmissivity values

10 – Arithmetic averaging of nodal transmissivity values

20 – Logarithmic averaging of nodal transmissivity values

30 – Logarithmic averaging of hydraulic conductivity, arithmetic averaging of saturated thickness

40 – Transmissivity/hydraulic conductivity values are specified between nodes, saturated thickness (if applicable) is arithmetically averaged.

LAYCON:

- 0 – confined – Transmissivity and storage coefficient of the layer are constant for the entire simulation
- 1 – unconfined – Transmissivity of the layer varies. It is calculated from the saturated thickness and hydraulic conductivity. The storage coefficient is constant. This layer type is valid only for layer 1.
- 2 – confined/unconfined – Transmissivity of the layer is constant. The storage coefficient may alternate between confined and unconfined values. Vertical flow from above is limited if the layer desaturates.
- 3 – confined/unconfined – Transmissivity of the layer varies. It is calculated from the saturated thickness and hydraulic conductivity. The storage coefficient may alternate between confined and unconfined values. Vertical flow from above is limited if the aquifer desaturates.
- 4 – unconfined variable hydraulic conductivity and specific yield with depth (VKD) – Transmissivity and specific yield of the layer varies. Transmissivity is calculated from the saturated thickness, the hydraulic conductivity, the hydraulic conductivity gradient factor, and the maximum hydraulic conductivity factor. The specific yield is calculated from the groundwater head, the primary storage coefficient, the storage gradient factor, and the maximum storage factor.**
- 5 – confined/unconfined variable hydraulic conductivity and specific yield with depth (VKD) – Transmissivity and specific yield of the layer varies. Transmissivity is calculated from the saturated thickness, the hydraulic conductivity, the hydraulic conductivity gradient factor, and the maximum hydraulic conductivity factor. The specific yield is calculated from the groundwater head, the secondary storage coefficient, the storage gradient factor, and the maximum storage factor. The storage coefficient may alternate between confined and unconfined values. Vertical flow from above is limited if the layer desaturates.**

TRPY is a one or three-dimensional array (depending on the value of **ITRPY** – see above) containing an anisotropy factor for each layer. It is the ratio of transmissivity or hydraulic conductivity (whichever is being used) along a column to transmissivity or hydraulic conductivity along a row. Set to 1.0 for isotropic conditions. This can be either a single array with one value per layer, or a separate array for each layer (if **ITRPY** is not **0**). If a single array is being used (**ITRPY** = **0**) only one array control record need be included for the entire array. If the value is the same for all layers, the entire array can be specified by setting LOCAT to 0 and setting CNSTNT to the value that applies to all layers. Read only if **ITRPY** is not **2**.

DELR is the cell width along rows. Read one value for each of the NCOL columns. This is a single array with one value for each column.

DELC is the cell width along columns. Read one value for each of the NROW rows. This is a single array with one value for each row.

Sf1 is a primary storage coefficient. Read only for a transient simulation (steady-state flag, ISS, is 0). For LAYCON equal to 1 or 4, Sf1 will always be specific yield, while for LAYCON equal to 2, 3 or 5 Sf1 will always be confined storage coefficient. For LAYCON equal to 0, Sf1 would normally be confined storage coefficient; however, a LAYCON value of 0 can also be used to simulate watertable conditions where drawdowns are expected to remain everywhere a small fraction of the saturated thickness, and where there is no layer above, or flow from above is negligible. In this case, specific yield values would be entered for Sf1. **If LAYCON is 4, the primary storage coefficient relates to the specific yield available from the lower (constant storage) zone.**

TranX is the transmissivity along rows. TranX is multiplied by TRPY to obtain transmissivity along columns (if ITRPY is not 2). Read only for layers where LAYCON is 0 or 2.

TranY is the transmissivity along columns. Read only for layers where LAYCON is 0 or 2 and ITRPY = 2.

HY is the hydraulic conductivity along rows. HY is multiplied by TRPY to obtain hydraulic conductivity along columns (if ITRPY is not 2). Read only for layers where LAYCON is 1, 3, 4 or 5. **(If ISS = 2, and LAYCON = 4 or 5, then Transmissivity is read into this array. If ISS = 3, and LAYCON = 4 or 5, then average hydraulic conductivity is read into this array).**

Hy-y is the hydraulic conductivity along columns. Read only for layers where LAYCON is 1, 3, 4 or 5 and ITRPY = 2. (If ISS = 2, and LAYCON = 4 or 5, then Transmissivity is read into this array. If ISS = 3, and LAYCON = 4 or 5, then average hydraulic conductivity is read into this array).

BOT is the elevation of the aquifer bottom. Read only for layers where LAYCON is 1, 3, 4 or 5.

Vcont is the vertical hydraulic conductivity divided by the thickness from a layer to the layer below. The value for a cell is the hydraulic conductivity divided by thickness for the material between the node in that cell and the node in the cell below. Because there is not a layer beneath the bottom layer, Vcont cannot be specified for the bottom layer.

sf2 is the secondary storage coefficient. Read only for layers where LAYCON is 2, 3 or 5, and only if the simulation is transient (steady-state flag, ISS, is 0). The secondary storage coefficient is always specific yield. **(If LAYCON = 5, the secondary storage coefficient relates to the specific yield available from the lower (constant storage) zone).**

TOP is the elevation of the aquifer top. Read only for layers where LAYCON is 2, 3 or 5.

WETDRY is a combination of the wetting threshold and a flag to indicate which neighbouring cells can cause a cell to become wet. If WETDRY < 0, only the cell below a dry cell can cause the cell to become wet. If WETDRY > 0, the cell below a dry cell and four horizontally adjacent cells can cause a cell to become wet. If WETDRY is 0, the cell cannot be wetted. The absolute value of WETDRY is the wetting threshold, when the sum of BOT and the absolute value of WETDRY at a dry cell is equalled or exceeded by the head at an adjacent cell, the cell is wetted. Read only if LAYCON is 1, 3, 4 or 5 and IWDFLG is not 0.

VMID is the elevation within the layer where hydraulic conductivity changes from being constant to varying with depth (point of inflection). Read only for layers where LAYCON is 4 or 5. (If ISS = 2 or 3 then the thickness of the upper (variable hydraulic conductivity) zone is read into this array).

VKGRAD is the hydraulic conductivity gradient (or gradient factor – depending on the value of IKBASE) applied to the upper (variable hydraulic conductivity) zone of an aquifer. Read only for layers where LAYCON is 4 or 5. If IKBASE is 0 it is multiplied by the hydraulic conductivity to give the hydraulic conductivity gradient. A positive value means that hydraulic conductivity increases linearly towards the top of the aquifer. Negative values can *not* be used to represent a linear decrease in hydraulic conductivity towards the top of the aquifer; if a zero or negative value is entered then both VKGRAD and VKMAX (below) are set to one. The hydraulic conductivity gradient only applies when the water table is in the upper (variable hydraulic conductivity) zone, ie, the head in the layer is above the VMID elevation.

VKMAX is the maximum hydraulic conductivity (or factor – depending on the value of IKBASE) applied to the upper (variable hydraulic conductivity) zone. Read only for layers where LAYCON is 4 or 5. If IKBASE is 0 it is multiplied by the hydraulic conductivity to give the maximum hydraulic conductivity.

VSMID is the elevation within the layer where storage changes from being constant to varying with depth (point of inflection). Read only for layers where LAYCON is 4 or 5 and if ISS is zero.

VSGRAD is the specific yield gradient (or gradient factor – depending on the value of IKBASE) applied to the upper (variable storage) zone of an aquifer. Read only if ISS is zero, for layers where LAYCON is 4 or 5. If IKBASE is 0 it is multiplied by the specific yield to give the specific yield gradient. A positive value means that specific yield increases linearly towards the top of the aquifer. Negative values can *not* be used to represent a linear decrease in specific yield towards the top of the aquifer; the storage calculations will be corrupted, leading to unrealistic results. The specific yield gradient only applies when the water table is in the upper (variable hydraulic conductivity) zone, ie, the head in the aquifer is above the VSMID elevation.

VSMAX is the maximum storage (or factor – depending on the value of IKBASE) applied to the upper (variable storage) zone. Read only if ISS is zero, for layers where LAYCON is 4 or 5. If IKBASE is 0 it is multiplied by the specific yield to give the maximum specific yield.

2.3.4 Summary of the inputs required for a VKD simulation

Table 2.2 Summary input instructions for VKD simulations

Input block	Steady State VKD	Alternative Steady State VKD (involves 2 simulations)	Time Variant VKD / VSD
1.	Set steady state flag (ISS) = 1	Set ISS = 2 (convert from specified transmissivity layers) or 3 (convert from specified hydraulic conductivity layers)	Set ISS = 0
2.	Layer type (LAYCON) = X4 or X5	LAYCON = X4 or X5	LAYCON = X4 or X5
3. or 3a.	Anisotropy ratio (TRPY) (if ITRPY is not 2)	TRPY (if ITRPY is not 2)	TRPY (if ITRPY is not 2)
4.	Cell width (DELR)	DELR	DELR
5.	Cell height (DELC)	DELC	DELC
6.	-	-	Sf1 (Specific yield of lower zone if LAYCON = 4. Confined storage coeff. if LAYCON = 5)
7.	-	-	-
7a.	-	-	-
8.	Hydraulic conductivity (HY) (of lower zone)	Steady State Transmissivity if ISS is 2, or average hydraulic conductivity if ISS is 3	HY (of lower zone)
8a.	Y-direction hydraulic conductivity (HY-y) of lower zone (if ITRPY = 2)	(if ITRPY = 2) Y-direction transmissivity (ISS=2), or hydraulic conductivity (ISS=3)	HY-y (if ITRPY = 2)
9.	Bottom elevation of layer (BOT)	BOT	BOT
10.	Vertical hydraulic conductivity over distance between layers (Vcont) (if not bottom layer)	Vcont (if not bottom layer)	Vcont (if not bottom layer)
11.	-	-	Sf2 (Sy of lower zone – if LAYCON = 5)
12.	Top elevation of layer (TOP) (if LAYCON = 5)	TOP (if LAYCON = 5)	TOP (if LAYCON = 5)

Table 2.2 Summary input instructions for VKD simulations (continued)

Input block	Steady State VKD	Alternative Steady State VKD (involves 2 simulations)	Time Variant VKD / VSD
13.	Wetting threshold (WETDRY) (if IWDFLG is not 0)	WETDRY (if IWDFLG is not 0)	WETDRY (if IWDFLG is not 0)
14.	Elevation of change in hydraulic conductivity (VMID)	VMID	VMID
15.	Hydraulic conductivity gradient factor (VKGRAD)	VKGRAD	VKGRAD
16.	Maximum hydraulic conductivity factor (VKMAX)	VKMAX	VKMAX
17.	-	-	Elevation of change in storage (VSMID)
18.	-	-	Storage gradient factor (VSGRAD)
19.	-	-	Maximum storage factor (VS MAX)

2.4 Module documentation for BCF package

The modified Block-Centred Flow Package (BCF-VKD1) has two new primary modules and three new submodules (highlighted in **bold** below). Modifications have also been made to all of the original modules. The relationships of the modules to the main program and to each other is shown in Figure 2.7.

Primary Modules

- BCF5AL Allocates space for data arrays.
 BCF5RP Reads all data needed by the package, invokes SBCF1N to reconcile input transmissive values with the IBOUND array, and calculates storage capacities and constant conductances.
 BCF5AD Set HOLD to BOT whenever a wettable cell is dry.
 BCF5FM Calculates all coefficients of the system of equations that are not constant and invokes SBCF5H to calculate horizontal branch conductances in partially saturated layers.
BCF5VK Writes new BCF, BAS and NAME files for 2nd initial conditions for VKD run. Initial heads from previous (specified T or K) run, top and bottom elevations calculated from heads and upper thicknesses, ISS set to 1, return to start of simulation.
BCF5OT Print and record internodal transmissivities.

Submodules

- SBCF5N Reconciles input transmissive values with the IBOUND array and calculates storage capacities and constant conductances. Invokes SBCF5C, A, L or I to calculate horizontal branch conductances for layers where transmissivity is constant.
 SBCF5H Calculates transmissivity for cells in layers where it depends on heads and invokes SBCF5C, A, L, U or I to calculate horizontal branch conductances.
 SBCF5C Calculates branch conductances using harmonic mean of cell transmissivities (activated by LAYAVG = 00).
 SBCF5A Calculates branch conductances using arithmetic mean of cell transmissivities (activated by LAYAVG = 10).
 SBCF5L Calculates branch conductances using logarithmic mean of cell transmissivities (activated by LAYAVG = 20).
 SBCF5U Calculates branch conductances using arithmetic mean saturated thickness and logarithmic mean hydraulic conductivity (activated by LAYAVG = 30).
SBCF5I Calculates branch conductances using internodal transmissivity (activated by LAYAVG = 40).
 SBCF5B Calculates flow between adjacent cells in a subregion of the grid.
 SBCF5S Calculates storage budget flow term for BCF.
 SBCF5F Calculates flow from constant-head cells.
B12DRI Routine to read 1 & 2-D real data input matrices and keep a record of the format.
SBCF5W Routine to write arrays to new BCF and BAS packages. Sets all values at no-flow and dry cells to zero, checks remaining values to see if they are all equal and prints the array record to the new files.

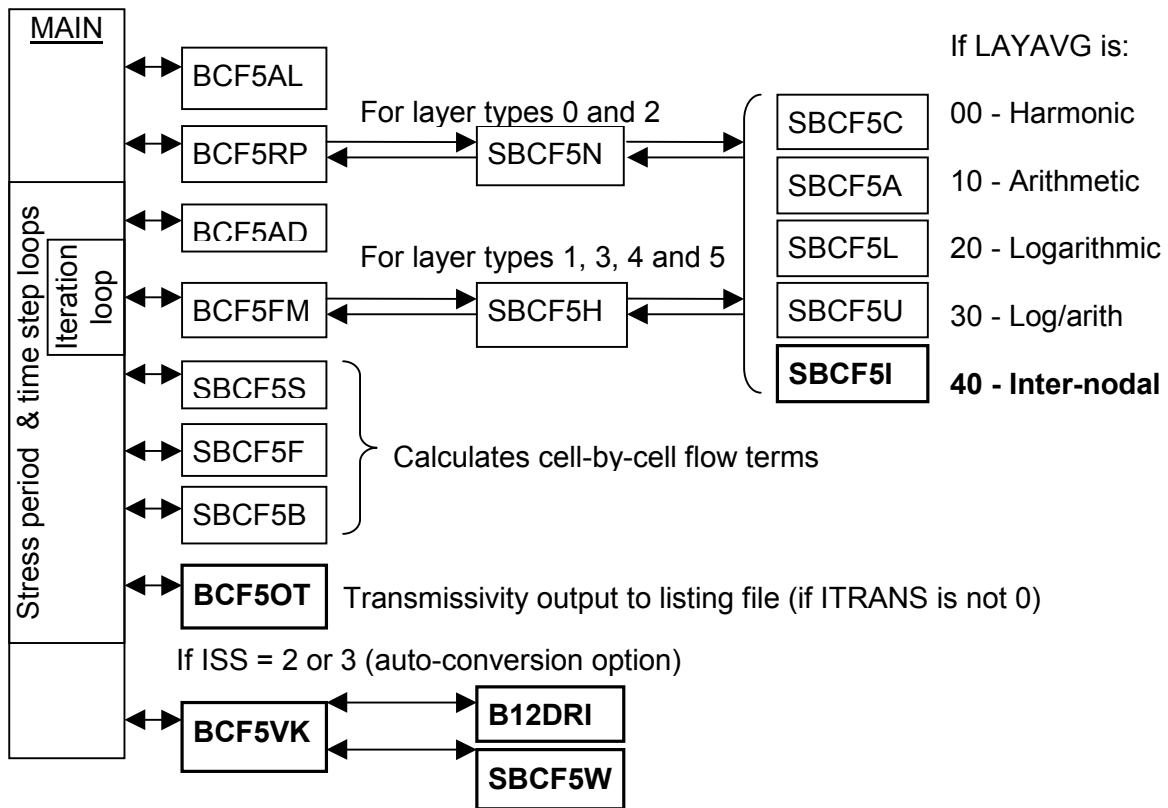
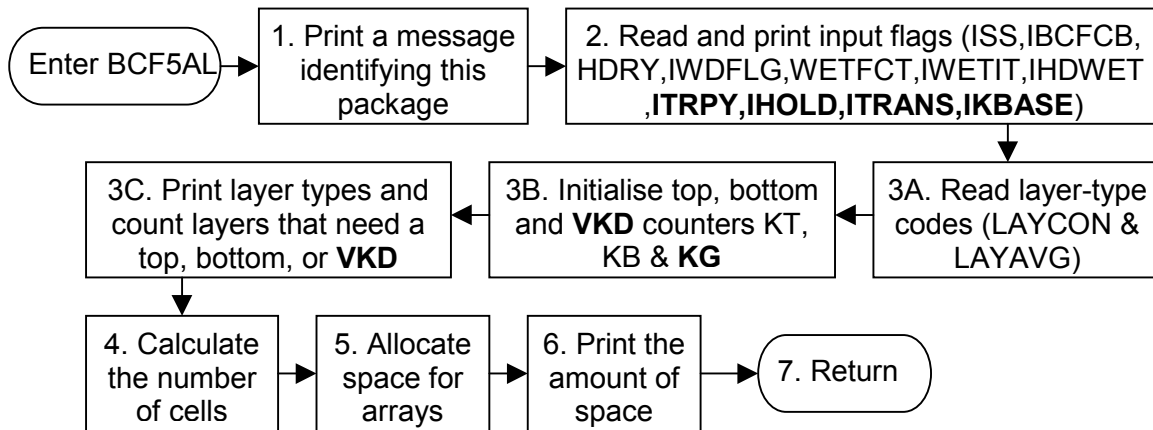


Figure 2.7 Relationship between the modules in the Block Centred Flow package

2.4.1 Changes to module BCF5AL

- Different title printed to listing file
- Read new input flags (ITRPY, IHOLD, ITRANS and IKBASE)
- Allow new layer types and interblock T code
- Allocate storage space for new arrays (expanded TRPY array, VKGRAD, VMID, VKMAX, VSGRAD, VSMID and VSMAX)

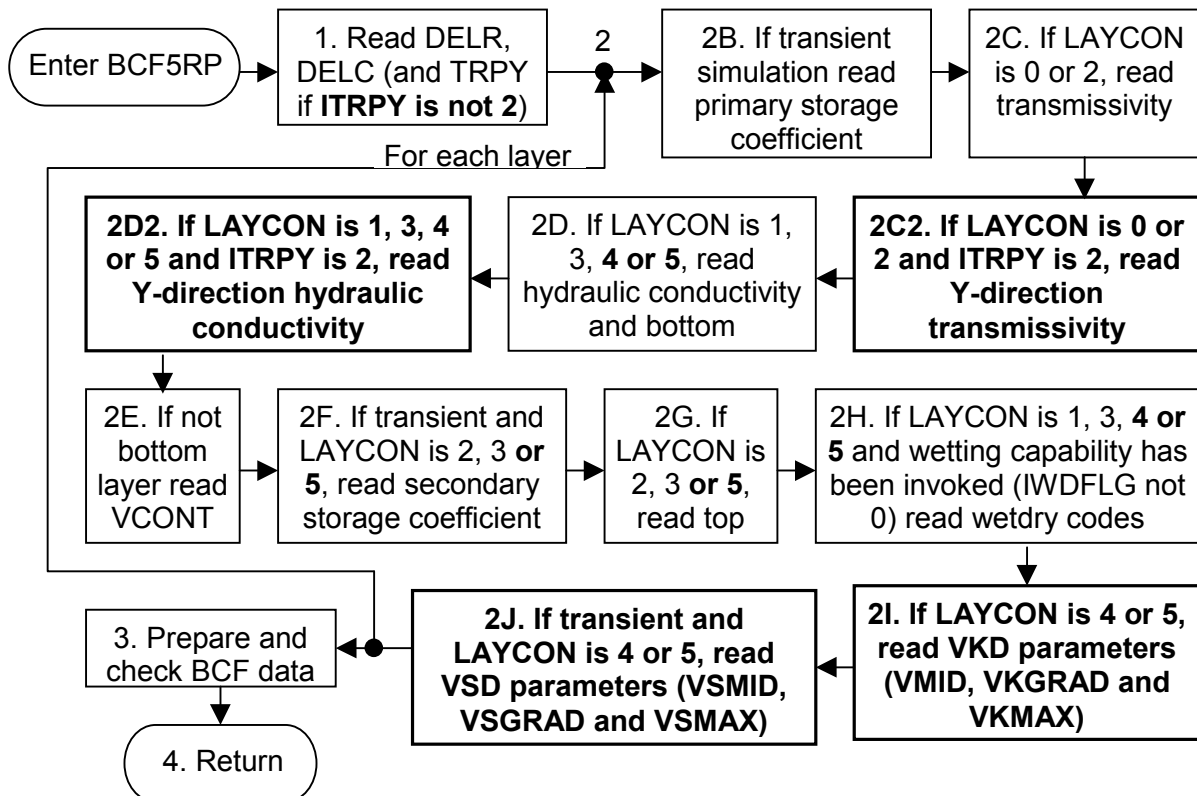
Flow Chart for module BCF5AL



2.4.2 Changes to module BCF5RP

- Add new array titles
- Allow new layer types
- Allow reading of arrays for spatially variable anisotropy
- Read new arrays (as for BCF5AL)

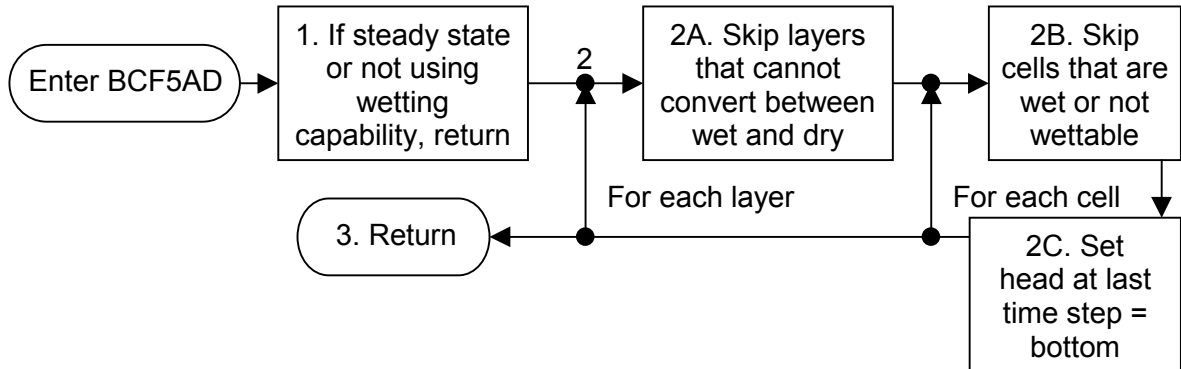
Flow chart for module BCF5RP



2.4.3 Changes to module BCF5AD

- Allow new layer types

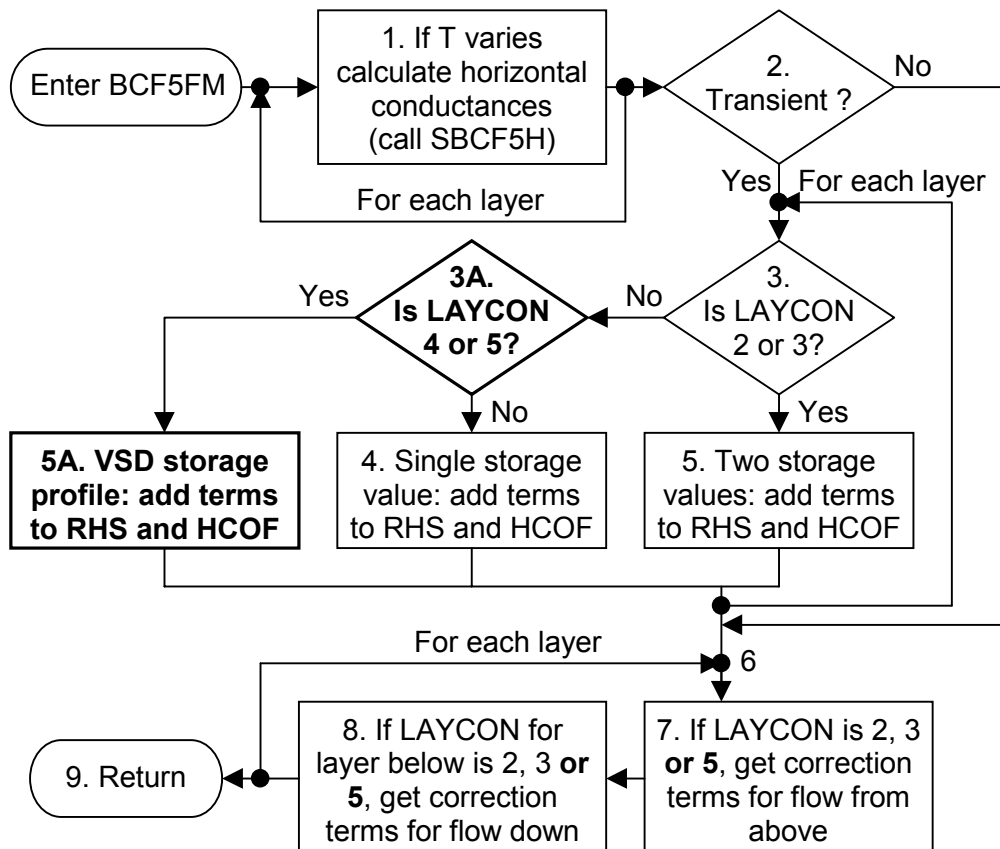
Flow chart for module BCF5AD



2.4.4 Changes to module BCF5FM

- Allow new layer types
- Include variable storage with depth calculations

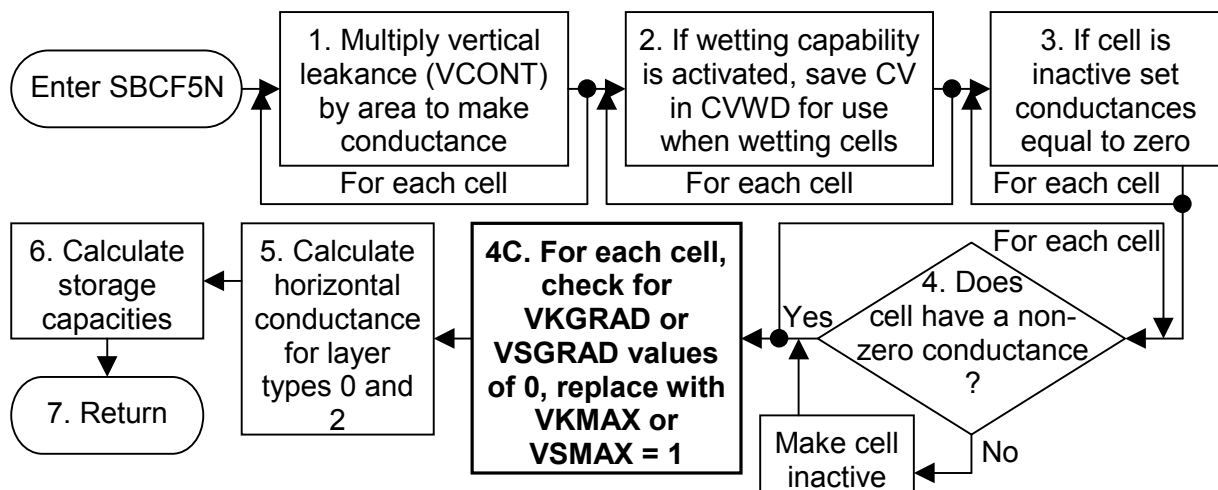
Flow chart for module BCF5FM



2.4.5 Changes to module SBCF5N

- Allow new layer types and interblock T code.
- Check all connecting branch conductances when using internodal transmissivity.
- Check for hydraulic conductivity gradient factor values of zero and replace with maximum hydraulic conductivity factor of one.
- Check for storage gradient factor values of zero and replace with maximum storage factor of one.

Flow chart for module SBCF5N



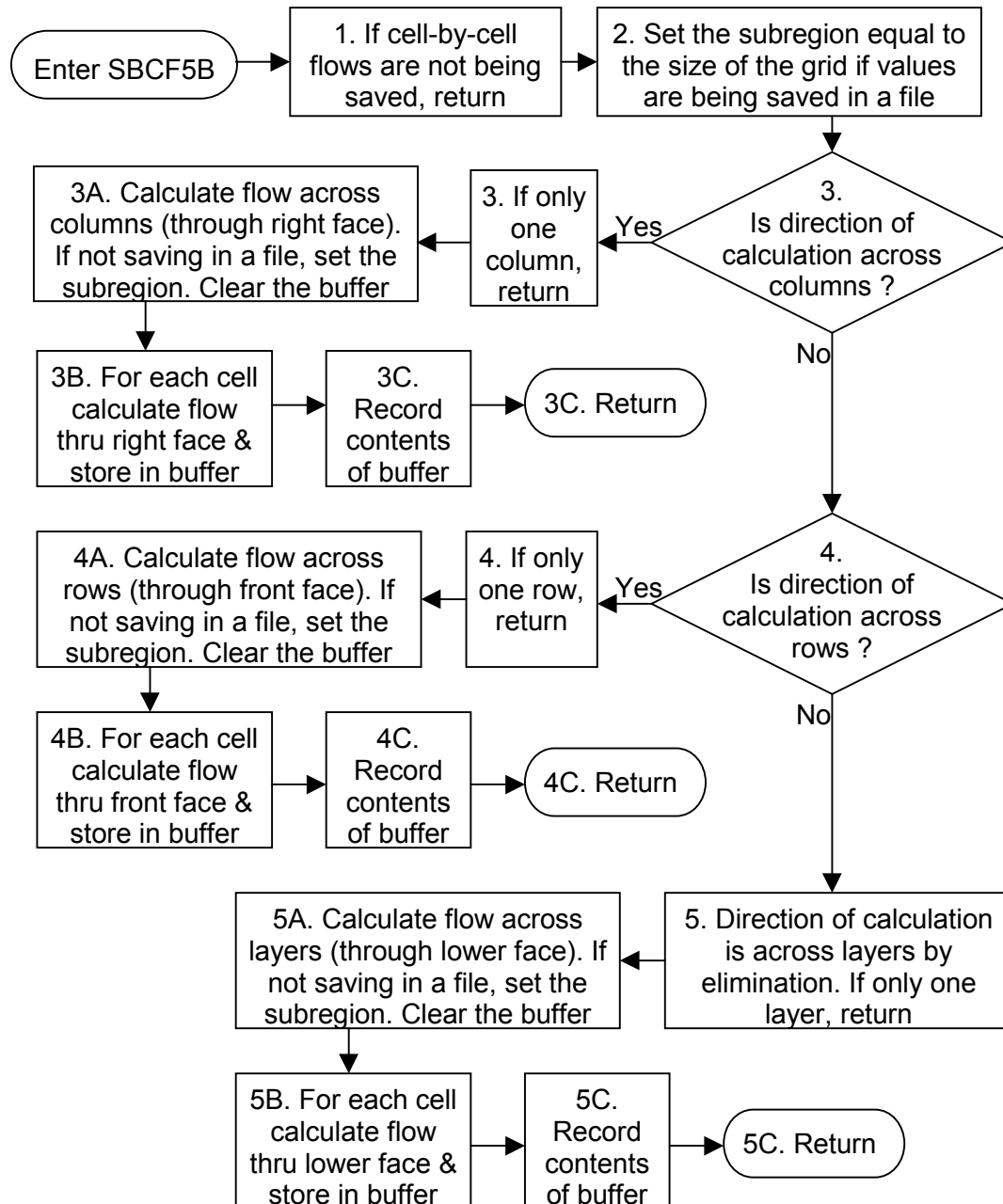
2.4.6 Changes to module SBCF5H

- Allow new layer types and interblock T code
- Allow explicit transmissivity option
- Include variable hydraulic conductivity with depth (VKD) calculations
- Include calculations for internodal transmissivity option (interblock T code)
- Allow spatially variable anisotropy

2.4.8 Changes to module SBCF5B

- Allow new layer types

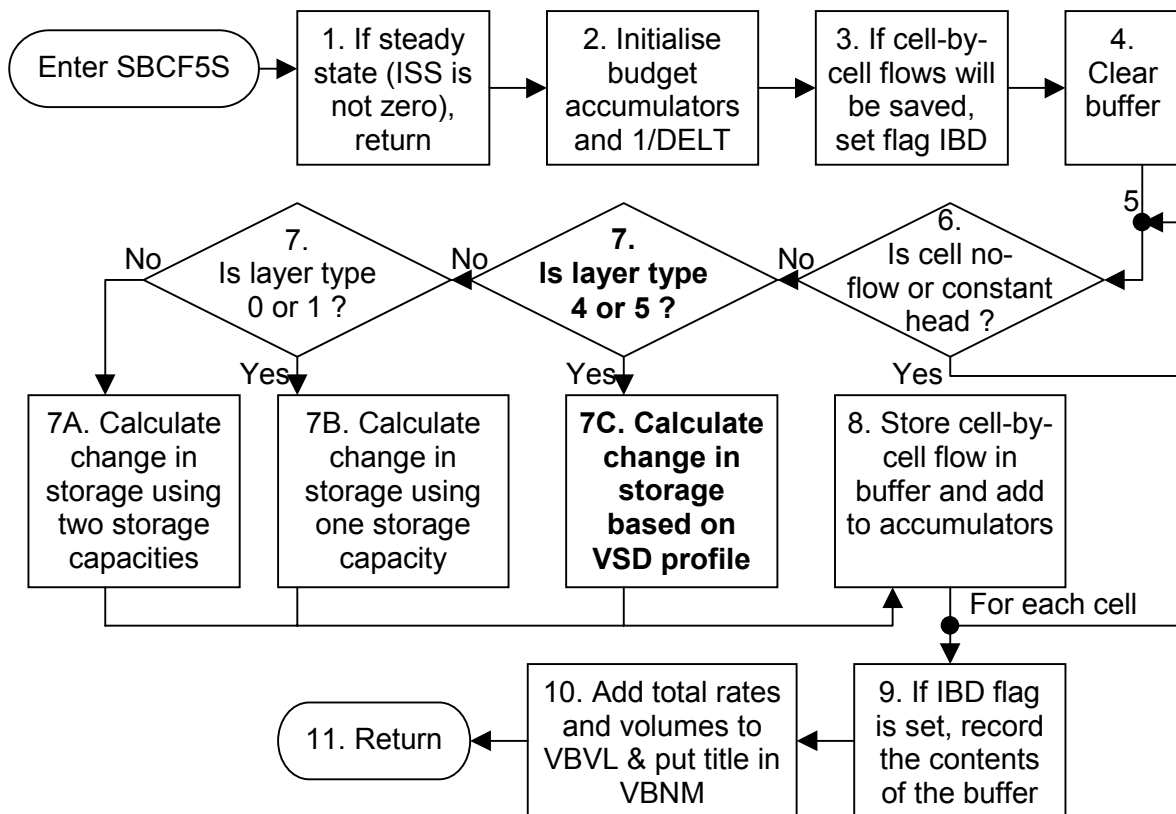
Flow chart for module SBCF5B



2.4.9 Changes to module SBCF5S

- Allow new layer types
- Include variable storage with depth calculations

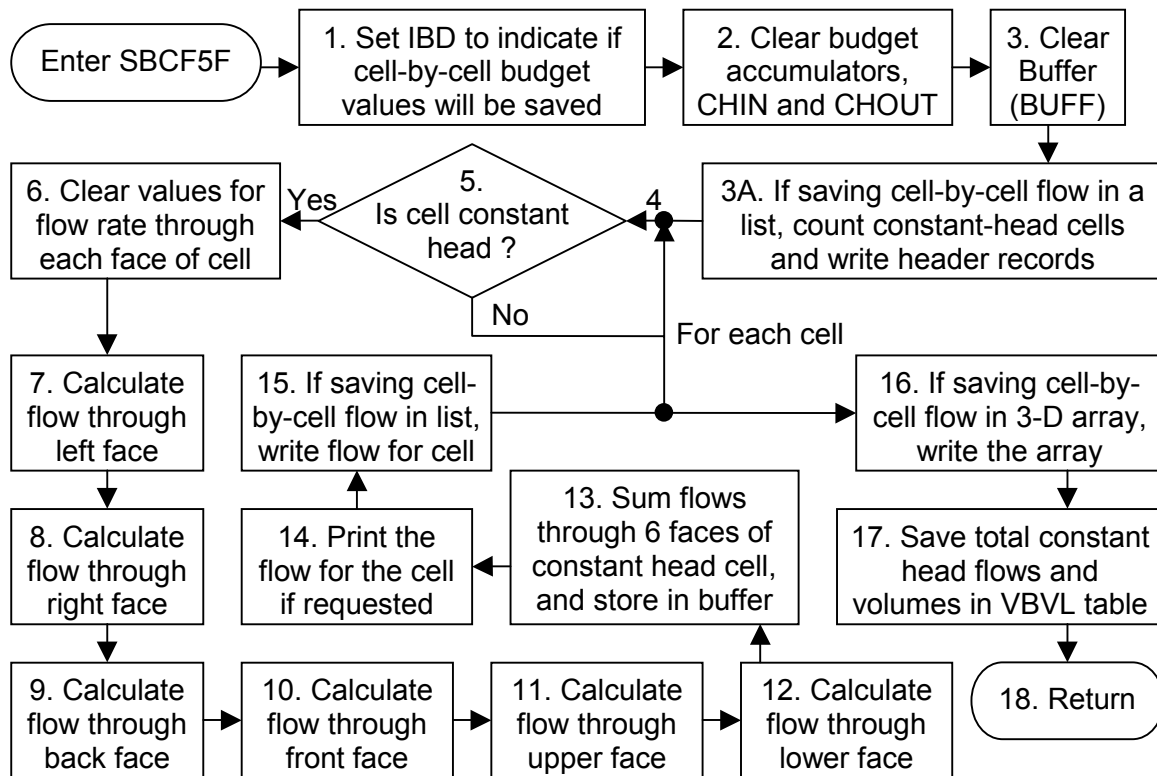
Flow chart for module SBCF5S



2.4.10 Changes to module SBCF5F

- Allow new layer types

Flow chart for module SBCF5F



2.4.11 Narrative for module BCF5VK

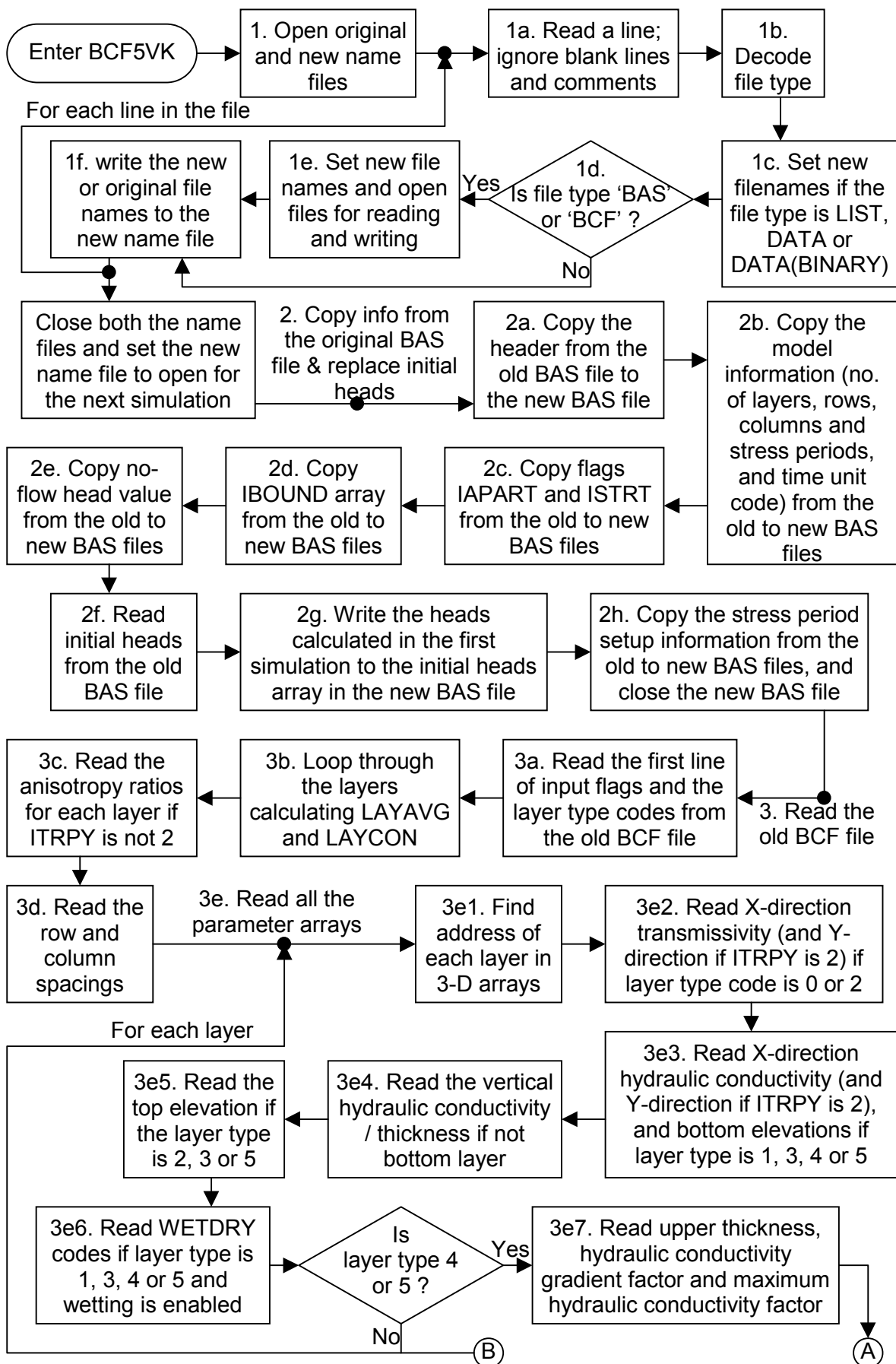
This module opens the name file, BAS and BCF files, reads the contents of the files, calculates the VKD parameters from the results of the first simulation (constant transmissivity or hydraulic conductivity simulation) and writes the new name, BAS and BCF files for the second simulation. Module BCF5VK is called by the main program after completion of the first simulation if the steady state flag (ISS) is 2 or 3. The module calls utility modules URWORD, U2DINT and ULAPRW, and the new BCF modules B12DRI and SBCF5W.

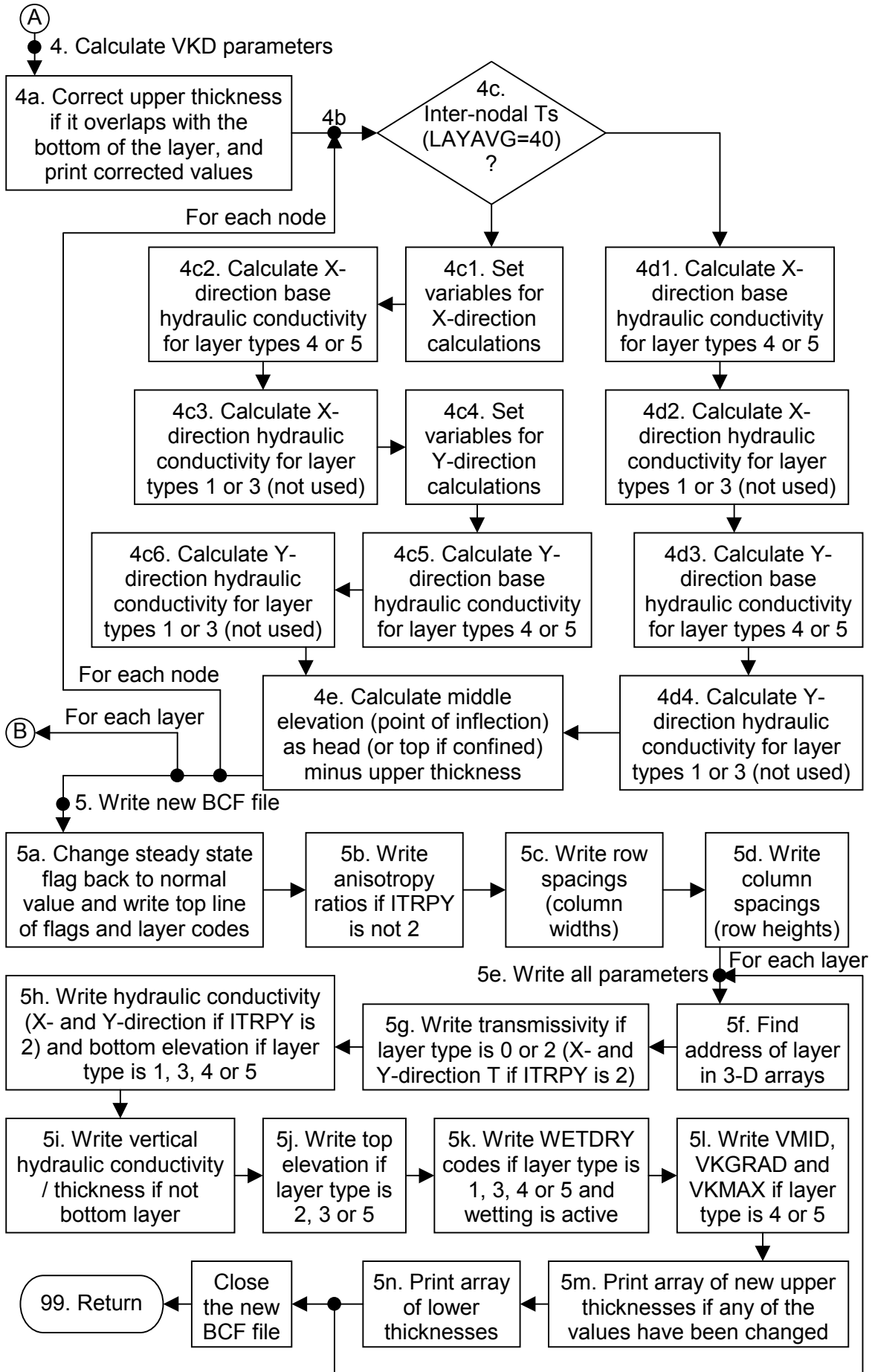
Module BCF5VK performs its functions in the following order:

1. Open original and new name files (code based on BAS module SBAS5O)
 - a. Read a line; ignore blank lines and comments (denoted by '#' character)
 - b. decode the file type
 - c. if the file type is 'LIST', 'DATA' or 'DATA(BINARY)' set new filenames
 - d. if the file type is 'BAS' or 'BCF' go to step 1e, otherwise go to step 1f
 - e. set new filenames for new BAS and BCF input files, and open the original and new files ready for reading and writing
 - f. write the new (or original) filenames to the new name file, return to step 1a if there is another line, otherwise close both the name files and set the new name file to open for the next simulation
2. Read the original BAS file and write a new BAS file with initial heads from the first simulation (code based on BAS modules BAS5DF, BAS5AL & BAS5RP):
 - a. Copy the text header from the old BAS file to the new BAS file
 - b. Copy the model information (number of layers, rows, columns and stress periods, and the time unit code) from the old BAS file to the new BAS file
 - c. Copy flags IAPART and ISTRT from the old BAS file to the new BAS file
 - d. Copy IBOUND array from the old BAS file to the new BAS file
 - e. Copy no-flow head value from the old BAS file to the new BAS file
 - f. Read initial heads from the old BAS file
 - g. Write the heads calculated in the first simulation to the initial heads array in the new BAS file
 - h. Copy the stress period setup information from the old BAS file to the new BAS file and close the new BAS file
3. Read the old BCF file (code based on BCF modules BCF5AL and BCF5RP)
 - a. Read ISS (steady-state flag), IBCFCB (flag for printing or unit number for recording cell-by-cell flow terms), HDRY (head at cells that convert to dry), wetting parameters, anisotropy option, explicit transmissivity calculation option, transmissivity output option, and layer type codes
 - b. Loop through layers calculating LAYAVG and LAYCON
 - c. Read the anisotropy ratios for each layer if ITRPY is not 2
 - d. Read the row and column spacings
 - e. Read all the parameters for each layer
 1. Find address of each layer in 3-D arrays
 2. Read X-direction transmissivity into array CC if layer type code is 0 or 2 (if ITRPY is 2, copy CC into array CR and read Y-direction transmissivity into array CC)
 3. Read X-direction hydraulic conductivity into array HY (and Y-direction hydraulic conductivity into array TRPY if ITRPY is 2) and bottom elevations into array BOT if layer type code is 1, 3, 4 or 5
 4. Read the vertical hydraulic conductivity / thickness into array CV if not bottom layer
 5. Read top elevation into array TOP if layer type code is 2, 3 or 5
 6. Read the WETDRY codes if layer type is 1, 3, 4 or 5 and wetting capability has been invoked (IWDFLG is not zero)

7. Read upper thickness into array VMID, hydraulic conductivity gradient factor into array VKGRAD, and maximum hydraulic conductivity factor into array VKMAX if layer type is 4 or 5
 4. Calculate VKD parameters (base hydraulic conductivities, anisotropy ratios, and middle elevations (point of inflection)) if layer type is 4 or 5
 - a. Correct upper thickness if it overlaps with the bottom of the layer (ie, if head minus upper thickness is less than the bottom elevation) and write corrected values to the output file for the first simulation
 - b. Loop through the cells in the layer calculating the VKD parameters:
 - c. Internodal transmissivity option:
 1. Set variables for X-direction calculations
 2. Calculate X-direction base hydraulic conductivities for layer types 4 or 5
 3. Calculate X-direction hydraulic conductivities for layer types 1 or 3 (not used)
 4. Set variables for Y-direction calculations
 5. Calculate Y-direction base hydraulic conductivities for layer types 4 or 5
 6. Calculate Y-direction hydraulic conductivities for layer types 1 or 3 (not used)
 - d. Block centred transmissivity option:
 1. Calculate X-direction base hydraulic conductivities for layer types 4 or 5
 2. Calculate X-direction hydraulic conductivities for layer types 1 or 3 (not used)
 3. Calculate Y-direction base hydraulic conductivities for layer types 4 or 5
 4. Calculate Y-direction hydraulic conductivities for layer types 1 or 3 (not used)
 - e. Calculate middle elevation (point of inflection, VMID) as head (or top if confined) minus upper thickness
 5. Write new BCF file
 - a. Change steady state flag (ISS) back to normal steady state value (1) and write top lines of flags and layer codes
 - b. Write anisotropy ratios if ITRPY is not 2
 - c. Write row spacings (column widths)
 - d. Write column spacings (row heights)
 - e. Write all parameters for each layer (f to n):
 - f. Find address of each layer in 3-D arrays
 - g. Write transmissivity if layer type is 0 or 2 (X- and Y-direction transmissivity if ITRPY is 2)
 - h. Write hydraulic conductivity (X- and Y-direction if ITRPY is 2) and bottom elevation if layer type is 1, 3, 4 or 5
 - i. Write vertical hydraulic conductivity / thickness if not bottom layer
 - j. Write top elevation if layer type is 2, 3 or 5
 - k. Write WETDRY codes if layer type is 1, 3, 4 or 5 and wetting capability has been invoked (IWDFLG is not 0)
 - l. Write middle elevation (point of inflection, VMID), hydraulic conductivity gradient factor (VKGRAD) and maximum hydraulic conductivity factor (VKMAX) if layer type is 4 or 5.
 - m. Write array of new upper thicknesses to the first output file if any of the values have been changed
 - n. Write array of lower thicknesses to the first output file and close the new BCF file
99. RETURN

Flow chart for module BCF5VK





List of variables for module BCF5VK

Variable	Range	Definition
AHDRY	Module	Character representation of HDRY variable (character*10)
ANAME	Module	DIMENSION(20) Labels for printout of input array (character*24 array)
ATMP	Module	Character representation of TMP variable (head at no-flow cells) (character*10)
AWETFCT	Module	Character representation of WETFCT variable (character*10)
BBOT	Module	Temporary variable to store bottom elevation for a node (real)
BOT	Package	DIMENSION (NCOL,NROW,NBOT), Elevation of bottom of each layer. (NBOT is the number of layers for which LAYCON is 1, 3, 4 or 5.) (real array)
BUFF	Global	DIMENSION (NCOL,NROW,NLAY), Buffer array with one element for each cell in the model. (real array)
CC	Package	DIMENSION (NCOL,NROW,NLAY), Conductance in the column direction. CC(J,I,K) contains conductance between nodes (J,I,K) and (J,I+1,K). (real array)
CR	Package	DIMENSION (NCOL,NROW,NLAY), Conductance in the row direction. CR(J,I,K) contains conductance between nodes (J,I,K) and (J+1,I,K). (real array)
CUNIT	Global	Character identifier for the packages listed in the name file (character*4)
CV	Package	DIMENSION (NCOL,NROW,NLAY-1), Conductance in the vertical direction. CV(J,I,K) contains conductance between nodes (J,I,K) and (J,I,K+1). (real array)
DELC	Package	DIMENSION (NROW), Cell dimension in the column direction. DELC(I) contains width of row I. (real array)
DELR	Package	DIMENSION (NCOL), Cell dimension in the row direction. DELC(J) contains width of column J. (real array)
FMTIN	Module	DIMENSION (15,200), Input format for each array in each layer (character*20 array)
FNAM2	Module	Filename of the new name file (character*80)
FNAME	Global	Filename of the original name file (character*80)
HDRY	Module	Head value assigned to nodes that have become unsaturated and hence inactive (real)
HEADNG	Module	Dimension (2), Heading printed on output to identify the problem. (character*80 array)
HHNEW	Module	Temporary variable to store groundwater head for a node (double precision)

Variable	Range	Definition
HNEW	Global	DIMENSION (NCOL,NROW,NLAY), Most recent estimate of groundwater head in each cell (double precision array)
HOLD	Global	DIMENSION (NCOL,NROW,NLAY), groundwater head in each cell from last time step (real array)
HY	Package	DIMENSION (NCOL,NROW,NBOT), Hydraulic conductivity of a cell. (NBOT is the number of layers for which LAYCON is 1, 3, 4 or 5.) (real array)
I	Module	Index (integer*4)
IAPART	Module	Flag set by user. (integer*4) = 0, arrays RHS and BUFFER will share space in the X array. ≠ 0, arrays RHS and BUFFER will not share space in the X array.
IBASOUT	Global	Unit number that the new BASic file will be written to (set to unit 94 in the main program) (integer*4)
IBCFCB	Module	Flag and a unit number. (integer*4) > 0, unit number on which cell-by-cell flow terms will be recorded whenever ICBCFL is set. = 0, cell-by-cell flow terms will not be printed or recorded < 0, flow from each constant head cell will be printed whenever ICBCFL is set
IBCFOUT	Global	Unit number that the new BCF file will be written to (set to unit 96 in the main program) (integer*4)
IBOUND	Global	DIMENSION (NCOL,NROW,NLAY), Status of each cell. (integer*4 array) < 0, constant-head cell = 0, inactive (no-flow) cell > 0, variable-head cell
IERR	Module	Flag indicating whether an upper thickness had to be reduced (integer*4)
IFREFM	Global	Flag indicating whether free format input files are being used (integer*4)
IHDWET	Module	Flag that determines which equation is used to calculate the initial head at cells that become wet (integer*4)
IHOLD	Module	Flag (integer*4) = 0, transmissivity is calculated using the current head ≠ 0, transmissivity is calculated using the head from the last time step
III	Module	Index (integer*4)
INAM1	Module	Location on a line of the name file of the start of a filename (integer*4)

Variable	Range	Definition
INAM2	Module	Location on a line of the name file of the end of a filename (integer*4)
INBAS	Global	Primary unit number from which input to the BAS package will be read (integer*4)
INBCF	Package	Unit number from which input to the BCF package will be read (integer*4)
INOUT	Global	Unit number that the new name file will be written to (set to unit 95 in the main program) (integer*4)
INUNIT	Global	Unit number on which the original name file will be opened (set to unit 99 in the main program) (integer*4)
IOUT	Global	Primary unit number for all printed output (integer*4)
IP	Module	Index (integer*4)
IRECL	Module	Record length of binary files opened as direct access (integer*4)
ISS	Module	Flag (integer*4) = 0, simulation is transient (time-variant) ≠ 0, simulation is steady state
ISTART	Module	Location on a line of the name file of the start of a word or number (integer*4)
ISTOP	Module	Location on a line of the name file of the end of a word or number (integer*4)
ISTRT	Module	Flag (integer*4) = 0, starting heads will be saved so that drawdown can be calculated ≠ 0, starting heads will not be saved
ITRANS	Module	Flag (integer*4) = 0, inter-nodal transmissivity values will not be written to the output file ≠ 0, inter-nodal transmissivity values will be written to the output file every time step
ITRPY	Module	Flag (integer*4) = 0, a single value of the anisotropy ratio will be used for each layer = 2, X- and Y-direction transmissivities or hydraulic conductivities will be specified for each cell in each layer ≠ 0 or 2, a value of the anisotropy ratio will be used for each cell in each layer
ITYP1	Module	Location on a line of the name file of the start of a file type code (integer*4)
ITYP2	Module	Location on a line of the name file of the end of a file type code (integer*4)
IU	Module	Temporary store for a unit number (integer*4)
IU1	Module	Temporary store for a unit number (integer*4)
IU2	Module	Temporary store for a unit number (integer*4)

Variable	Range	Definition
IWDFLG	Module	Flag (integer*4) = 0, rewetting capability is not active ≠ 0, rewetting capability is active
IWETIT	Module	Iteration interval for attempting to wet cells (integer*4)
IXSEC	Global	Flag (integer*4) = 0, Model is not a cross section ≠ 0, Model is a cross section
J	Module	Index (integer*4)
JP	Module	Index (integer*4)
K	Module	Index for layers (integer*4)
KB	Module	Counter for the number of layers for which the bottom elevation is needed (LAYCON = 1, 3, 4 or 5) (integer*4)
KG	Module	Counter for the number of layers for which the gradient factor is needed (LAYCON = 4 or 5) (integer*4)
KK	Module	Temporary variable set equal to K (integer*4)
KT	Module	Counter for the number of layers for which the top elevation is needed (LAYCON = 2, 3, 4 or 5) (integer*4)
LAYAVG	Package	DIMENSION (200) Layer averaging code (integer*4 array): = 00, Harmonic averaging = 10, Arithmetic averaging = 20, Logarithmic averaging = 30, Log/arithmetic averaging = 40, Inter-nodal values used directly
LAYCON	Package	DIMENSION (200) Layer type code (integer*4 array): = 0, layer strictly confined = 1, Layer strictly unconfined = 2, Layer confined/unconfined (transmissivity is constant) = 3, Layer confined/unconfined (transmissivity depends on head)
LINE	Module	Line read from name file (character*80)
LINE1	Module	Temporary character string (character*80)
LINE2	Module	Temporary character string (character*80)
LLOC	Module	Counter specifying current position in a character string (integer*4)
N	Module	Temporary integer value (integer*4)
NCOL	Global	Number of columns in the grid (integer*4)
NLAY	Global	Number of layers in the grid (integer*4)
NPER	Global	Number of stress periods in the simulation (integer*4)
NROW	Global	Number of rows in the grid (integer*4)
NSTP	Module	Number of time steps in the current stress period (integer*4)

Variable	Range	Definition
PERLEN	Module	Length of the stress period (real)
PERLENNSTPTSMUL T	Module	Character representation of the variables PERLEN, NSTP and TSMULT (character*30)
R	Module	Temporary real value (real)
SC1	Package	DIMENSION (NCOL,NROW,NLAY), Primary storage capacity for each cell (S*DELC*DELR) (real array)
SC2	Package	DIMENSION (NCOL,NROW,NTOP), Secondary storage capacity for each cell (real array) (NTOP is the number of layers for which LAYCON = 2, 3 or 5)
T	Module	Temporary variable for storing a transmissivity value for a cell (real)
TMP	Module	Temporary variable for storing the value of head for no-flow cells (real)
TOP	Package	DIMENSION (NCOL,NROW,NTOP), Elevation of the top of the layers (real array) (NTOP is the number of layers for which LAYCON = 2, 3 or 5)
TRPY	Package	DIMENSION (NCOL,NROW,NLAY), Anisotropy ratio: ratio of transmissivity in the column direction to transmissivity in the row direction (real array)
TSMULT	Module	Multiplier to get from one time step length to the next (real)
TTOP	Module	Temporary variable to store top elevation for a node (real)
VKGRAD	Package	DIMENSION (NCOL,NROW,NGRAD), Hydraulic conductivity gradient factor for each cell (NGRAD is the number of layers for which LAYCON = 4 or 5) (real array)
VKMAX	Package	DIMENSION (NCOL,NROW,NGRAD), Maximum hydraulic conductivity factor for each cell (NGRAD is the number of layers for which LAYCON = 4 or 5) (real array)
VMID	Package	DIMENSION (NCOL,NROW,NGRAD), Elevation of the point of inflection for each cell (NGRAD is the number of layers for which LAYCON = 4 or 5) (real array)
VVKGRAD	Module	Temporary variable to store the hydraulic conductivity gradient factor for a cell (real)
VVKMAX	Module	Temporary variable to store the maximum hydraulic conductivity factor for a cell (real)
VVMID	Module	Temporary variable to store the elevation of the point of inflection for a cell (real)

Variable	Range	Definition
WETDRY	Package	DIMENSION (NCOL,NROW,NLAY), Wetting threshold and flag (real array) < 0, only the cell below a dry cell can cause the cell to become wet > 0, the cell below a dry cell and four horizontally adjacent cells can cause a cell to become wet = 0, the cell cannot be wetted
WETFCT	Module	Factor that is included in the calculation of the head that is initially established at a cell when it is converted from dry to wet (real)

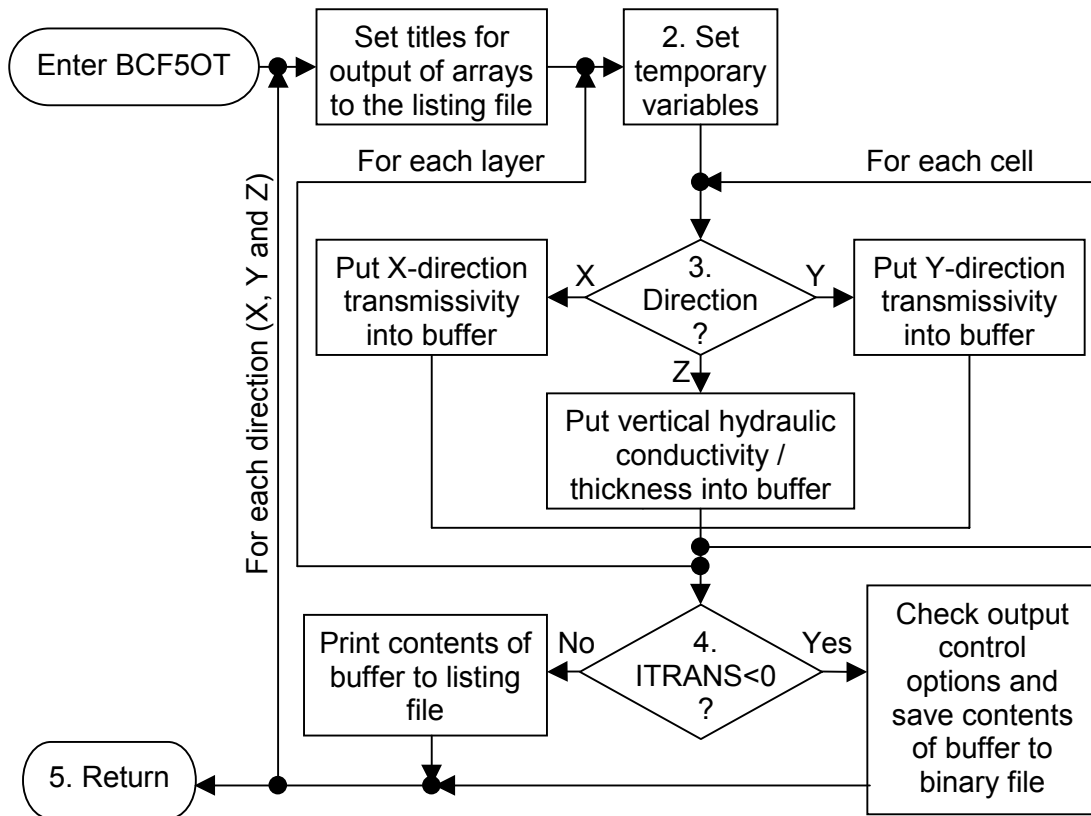
2.4.12 Narrative for module BCF5OT

This module prints arrays of X- and Y-direction interblock transmissivities, and vertical hydraulic conductivity/thickness to the listing file or a binary output file. Module BCF5OT is called by the main program after each time step if the flag ITRANS is not zero. If ITRANS is positive, the module writes transmissivity values to the listing file using utility modules ULAPRS or ULAPRW depending on the value of IHEDFM specified in the output control file (McDonald & Harbaugh, 1988, pp. 4-14 to 4-15). If ITRANS is negative, the module saves transmissivity values to a binary output file denoted by the negative value of ITRANS, using the utility modules ULASAV or ULASV2.

Module BCF5OT performs its functions in the following order:

0. Loop through X, Y and Z directions and set titles to write to listing file for each array
1. Loop through each layer
2. Set temporary variables
3. Loop through all cells putting X- or Y-direction transmissivity, or vertical hydraulic conductivity / thickness into the buffer array
4. Check sign of ITRANS and either print the contents of the buffer array to the listing file, or save them to a binary file (subject to output control specified for heads) and loop back for next layer
5. Return

Flow chart for module BCF5OT



List of variables for module BCF5OT

Variable	Range	Definition
BUFF	Global	DIMENSION (NCOL,NROW,NLAY), Buffer array with one element for each cell in the model. (real array)
CC	Package	DIMENSION (NCOL,NROW,NLAY), Conductance in the column direction. CC(J,I,K) contains conductance between nodes (J,I,K) and (J,I+1,K). (real array)
CHEDFM	Global	Character expression denoting format code for printed head output
CR	Package	DIMENSION (NCOL,NROW,NLAY), Conductance in the row direction. CR(J,I,K) contains conductance between nodes (J,I,K) and (J+1,I,K). (real array)
CV	Package	DIMENSION (NCOL,NROW,NLAY-1), Conductance in the vertical direction. CV(J,I,K) contains conductance between nodes (J,I,K) and (J,I,K+1). (real array)
DELC	Package	DIMENSION (NROW), Cell dimension in the column direction. DELC(I) contains width of row I. (real array)
DELR	Package	DIMENSION (NCOL), Cell dimension in the row direction. DELC(J) contains width of column J. (real array)
I	Module	Index (integer*4)
IBOUND	Global	DIMENSION (NCOL,NROW,NLAY), Status of each cell. (integer*4 array) < 0, constant-head cell = 0, inactive (no-flow) cell > 0, variable-head cell
IHEDFM	Global	Code for format in which head should be printed (same format used for transmissivity values) (integer*4)
IOFLG	Output Control module	DIMENSION (NLAY,4), Flags to control printing and recording of head and drawdown for each layer (NLAY,1) ≠ 0, heads will be printed (NLAY,2) ≠ 0, drawdown will be printed (NLAY,3) ≠ 0, heads and transmissivities will be recorded (NLAY,4) ≠ 0, drawdown will be recorded
IOUT	Global	Primary unit number for all printed output (integer*4)
ITRAN	Module	Direction index (integer*4)

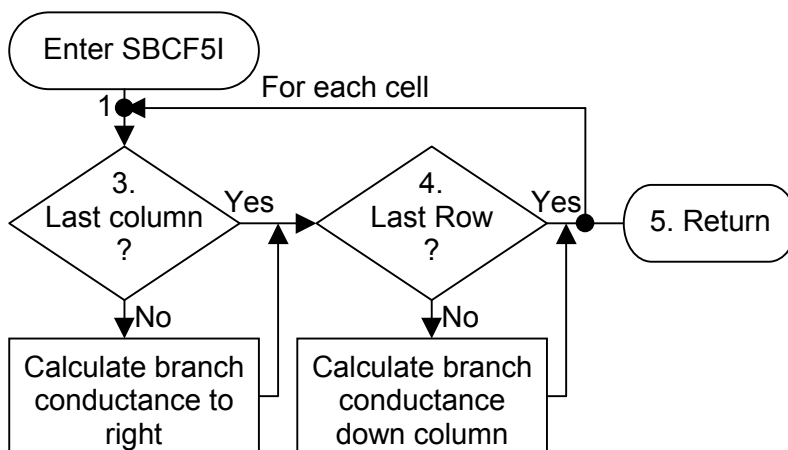
Variable	Range	Definition
ITRANS	Package	Flag (integer*4) = 0, inter-nodal transmissivity values will not be written to the output file > 0, inter-nodal transmissivity values will be written to the output file every time step < 0, inter-nodal transmissivity values will be saved to a binary output file for every time step specified in the Output Control file (uses same flag as for head save)
ITRPY	Package	Flag (integer*4) = 0, a single value of the anisotropy ratio will be used for each layer = 2, X- and Y-direction transmissivities or hydraulic conductivities will be specified for each cell in each layer ≠ 0 or 2, a value of the anisotropy ratio will be used for each cell in each layer
IXSEC	Package	Flag (integer*4) = 0, Model is not a cross section ≠ 0, Model is a cross section
J	Module	Index (integer*4)
K	Module	Index for layers (integer*4)
KK	Module	Index (integer*4)
KL	Module	Index (integer*4)
KPER	Global	Stress period counter (integer*4)
KSTP	Global	Time step counter (integer*4). Reset at the start of each stress period
LBHDSV	Global	Flag denoting whether head save (and transmissivity) files will be labelled
NCOL	Global	Number of columns in the grid (integer*4)
NLAY	Global	Number of layers in the grid (integer*4)
NROW	Global	Number of rows in the grid (integer*4)
PERTIM	Global	Elapsed time during the current stress period
TEXT	Module	Title printed to the listing file to identify the array (character*16)
TOTIM	Global	Elapsed time in the simulation
TRPY	Package	DIMENSION (NCOL,NROW,NLAY), Anisotropy ratio: ratio of transmissivity in the column direction to transmissivity in the row direction (real array)
YX	Module	Temporary store for the anisotropy ratio (real)

2.4.13 Narrative for module SBCF5I

The module SBCF5I calculates horizontal branch conductances for a layer from inter-nodal transmissivity and cell dimensions. It is called by submodules SBCF5N and SBCF5H. The module is based on module SBCF5A and performs the same functions as those described for the modules in Section 2.4.7.

- 1) Process cells one at a time calculating branch conductances from that cell to the one on the right and the one in front.
- 2) This step has been removed as there is no need to check for transmissivity values of zero.
- 3) If there is a cell to the right, calculate the branch conductance (CR) along the row.
- 4) If there is a cell in front, calculate the conductance (CC) along the column.
- 5) Return.

Flow chart for module SBCF5I



List of variables for module SBCF5I

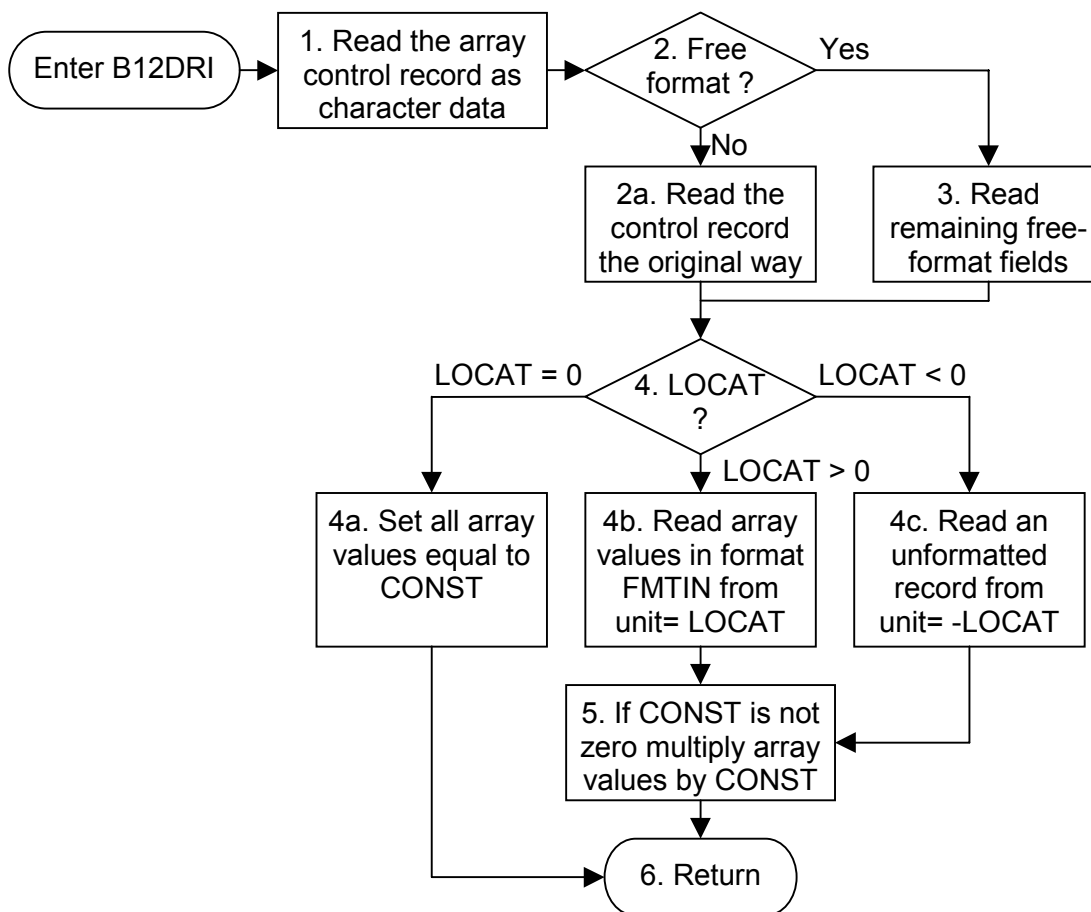
Variable	Range	Definition
CC	Package	DIMENSION (NCOL,NROW,NLAY), Conductance in the column direction. CC(J,I,K) contains conductance between nodes (J,I,K) and (J,I+1,K). (real array)
CR	Package	DIMENSION (NCOL,NROW,NLAY), Conductance in the row direction. CR(J,I,K) contains conductance between nodes (J,I,K) and (J+1,I,K). (real array)
DELC	Package	DIMENSION (NROW), Cell dimension in the column direction. DELC(I) contains width of row I. (real array)
DELR	Package	DIMENSION (NCOL), Cell dimension in the row direction. DELC(J) contains width of column J. (real array)
I	Module	Index (integer*4)
ITRPY	Package	Flag (integer*4) = 0, a single value of the anisotropy ratio will be used for each layer = 2, X- and Y-direction transmissivities or hydraulic conductivities will be specified for each cell in each layer ≠ 0 or 2, a value of the anisotropy ratio will be used for each cell in each layer
J	Module	Index (integer*4)
K	Package	Index for layers (integer*4)
NCOL	Global	Number of columns in the grid (integer*4)
NLAY	Global	Number of layers in the grid (integer*4)
NROW	Global	Number of rows in the grid (integer*4)
T1	Module	Temporary store for conductance in the row direction (real)
T2	Module	Temporary store for conductance in the column direction (real)
TRPY	Package	DIMENSION (NCOL,NROW,NLAY), Anisotropy ratio: ratio of transmissivity in the column direction to transmissivity in the row direction (real array)
YX	Module	Temporary store for the anisotropy ratio (real)
ZERO	Module	Variable set to value of zero (real)

2.4.14 Narrative for module B12DRI

The module B12DRI reads values for a two-dimensional real array. It is based on module U2DREL in the utilities package, but has been modified to suppress printing of arrays to the listing file and to enable format codes to be stored for future use. The module B12DRI is called from module BCF5VK and calls the utility routine URWORD. It performs its functions in the following order:

1. Read the array control record as character data.
2. Look for alphabetic word that indicates that the record is free format. Set a flag specifying if free format or fixed format.
- 2a. If a recognised word was not found, read the control record the original way (LOCAT, CONST, FMTIN, IPRN).
3. For free format control record, read remaining fields.
4. Test LOCAT to see how to define array values.
 - a. LOCAT=0; set all array values equal to CONST and return.
 - b. LOCAT>0; read formatted records using format FMTIN.
 - c. LOCAT<0; read unformatted record containing array values.
5. If CONST is not zero then multiply array values by CONST.
6. Return

Flow chart for module B12DRI



List of variables for module B12DRI

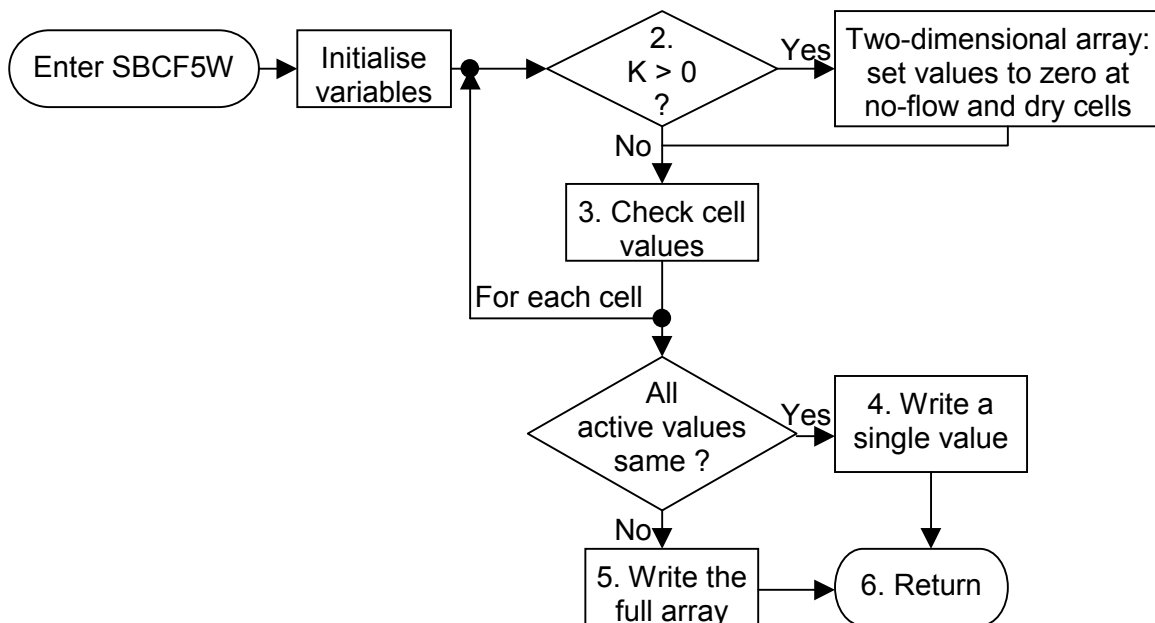
Variable	Range	Definition
A	Module	DIMENSION (JJ,II), Input array (real array)
CNTRL	Module	Character string used to read array control record (character*80)
CONST	Module	Constant to which all array values are set if LOCAT is equal to zero or by which all array values are multiplied if LOCAT is not equal to zero (real)
FMTIN	Module	Format under which array values will be read (character*20)
FNAME	Module	Filename of file containing array if OPEN/CLOSE option is used to read array (character*80)
I	Module	Index for rows (integer*4)
ICLOSE	Module	Flag used to specify whether an OPEN/CLOSE file has been opened (integer*4)
ICOL	Module	Index for position along text string CNTRL (integer*4)
IFREE	Module	Flag used to indicate if free format is being used (integer*4)
II	Module	Number of rows (integer*4)
IN	Module	Unit number from which the array control record will be read (integer*4)
IOUT	Global	Primary unit number for all printed output (integer*4)
IP	Module	Flag to indicate whether array values are written to the output file (0 suppresses output) (integer*4)
IPRN	Module	Code for format to be used when printing the arrays (not used in this routine) (integer*4)
ISTART	Module	Location on a line of the name file of the start of a word or number (integer*4)
ISTOP	Module	Location on a line of the name file of the end of a word or number (integer*4)
J	Module	Index for columns (integer*4)
JJ	Module	Number of columns (integer*4)
LOCAT	Module	Location of values to fill in the array (integer*4) < 0, read an unformatted record containing the array values = 0, set all the array values equal to constant (CONST) > 0, read the formatted records containing the array values
N	Module	Temporary integer value (integer*4)
NUNOPN	Module	Unit number for OPEN/CLOSE files (99) (integer*4)
R	Module	Temporary real value (real)

2.4.15 Narrative for module SBCF5W

The module SBCF5W writes values for a two-dimensional real array that can be read by the array readers in MODFLOW (including the array-control record with a specified format). It is called from module BCF5VK to write the arrays for the new BAS and BCF packages when the auto-conversion option is activated. It performs its functions in the following order:

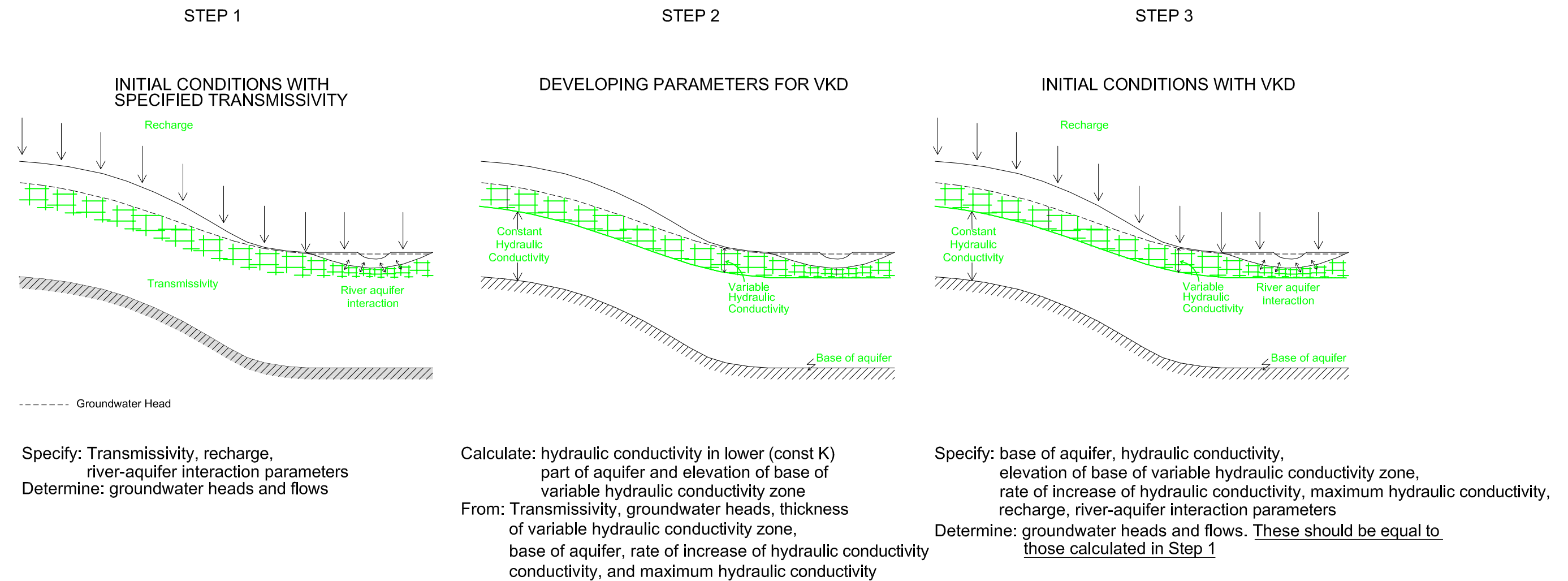
0. Initialise variables.
1. Loop through all the cells in the layer.
2. If $K > 0$ then 2-d array, set values to zero at dry/no-flow cells (this avoids the likelihood of cells with unrealistic VKD parameters becoming active due to rewetting in subsequent simulations).
3. Check if all the active values in the array are the same.
4. If all active values are the same write a single value.
5. Otherwise write out the full array.
6. Return.

Flow chart for module SBCF5W



List of variables for module SBCF5W

Variable	Range	Definition
A	Module	DIMENSION (JJ,II), Output array (real array)
ALAST	Module	Temporary store for comparing values in an array (real)
ANAME	Module	Label for printout of output array (character*24)
FMT	Module	Format that will be used to write arrays (character*20)
HDRY	Package	Head value assigned to nodes that have become unsaturated and hence inactive (real)
HNEW	Global	DIMENSION (NCOL,NROW,NLAY), Most recent estimate of groundwater head in each cell (double precision array)
I	Module	Index for rows (integer*4)
IBCFOUT	Module	Unit number of the file that arrays will be written to (integer*4)
IBOUND	Global	DIMENSION (NCOL,NROW,NLAY), Status of each cell. (integer*4 array) < 0, constant-head cell = 0, inactive (no-flow) cell > 0, variable-head cell
ICONST	Module	Flag used to indicate whether all active values in the array are the same (integer*4)
IFIRST	Module	Flag used to determine whether the first active value in the array has been read (integer*4)
INBCF	Package	Unit number to write in the array control record (integer*4)
J	Module	Index for columns (integer*4)
K	Module	Layer number (integer*4)
NCOL	Package	Number of columns (integer*4)
NLAY	Package	Number of layers (integer*4)
NROW	Package	Number of rows (integer*4)



3 STREAM PACKAGE

3.1 Introduction

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

The processes represented by the stream package are given below prior to the description of the new features.

Streams that interact with the modelled aquifer are divided into reaches and segments. A segment is a stream or diversion in which stream flow from surface sources are added at the beginning of the segment or subtracted (in the case of a diversion) at the end of the segment. A reach is the part of a segment that corresponds to an individual cell in the finite-difference grid used to simulate groundwater flow in the aquifer. Segments are numbered sequentially from the farthest upstream segment to the last downstream segment, as are reaches within each segment. Both must also be read into the program in sequential order.

Streamflow is accounted for by specifying flow for the first reach in each segment that enters the modelled area and then computing streamflow to adjacent downstream reaches in each segment as equal to inflow in the upstream reach plus or minus leakage from or to the aquifer in the upstream reach. The accounting scheme used assumes that streamflow entering a stream reach is instantly available to downstream reaches. This assumption is generally reasonable because of the relatively slow rates of groundwater flow.

Streamflow into a segment that is formed from tributary streams is computed by adding the outflows from the last reach in each of the specified tributary segments. If a segment is a diversion, then the specified flow into the first reach of the segment is subtracted from flow in the main stream. However, if the specified flow of the diversion is greater than the flow out of the segment from which flow is to be diverted, then no flow is diverted from that segment.

Reaches in a segment are permitted to go dry whenever downward leakage to the aquifer exceeds stream inflow into the reach. The downstream reaches also go dry (streamflow into the downstream reaches is zero) and leakage into the aquifer is not permitted. Upward leakage (from the aquifer) is permitted even when there is no streamflow in a reach. This happens when the head in the aquifer exceeds the top of the streambed in the dry reach. Flow in the stream resumes and water may leak downwards back into the aquifer again in downstream reaches.

3.2 Conceptualisation and implementation of new features

The following discussion of the conceptualisation and implementation of the new features included in the stream package is divided into three sections: specified discharges or abstractions at any stream cell, tributary inflows at any stream cell, and a small correction to cell-by-cell stream flow output.

3.2.1 *Specified discharges or abstractions at any stream cell*

The original version of the stream package allows a specified inflow rate, i.e. a discharge, to be assigned only at the first reach (ie, first cell) of a segment, and does not allow surface water abstraction.. The input format includes a column for this flow rate for all stream reaches, but the value was ignored in all but the first reach in each segment. It looks as if the original version of the package was intended to allow inflows at any cell but was later changed.

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

3.2.2 *Tributary inflows at any stream cell*

The original version of the stream package allows tributary inflows to be assigned only at the first reach (ie, first cell) of a segment. The second modification of the stream package allows tributary inflows to be specified for any reach in a segment. This modification allows a major river to be specified with a single segment number, with tributary inflows from smaller streams at various points along its length. This change has been made to make pre- and post-processing easier. Setting the new flag (ISWABS) to a positive value activates the option. It may be noticed that this modification applies only to tributary inflows and not to diversions.

3.2.3 *Small correction to cell-by-cell stream flow output*

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

3.3 Input instructions

3.3.1 Summary of new options

This new version of the MODFLOW modelling code allows two new options to be set (shown in **bold**) in the input instructions for the stream package. The new code should still be compatible with old MODFLOW input files (versions up to MODFLOW-96). The new options included are:

- **Allow surface water discharges and abstractions to be specified in any reach -** set **ISWABS <> 0** and specify positive (discharges) or negative (abstractions) values for the Flow into each reach
- **Allow tributary inflows to be specified in any reach -** set **ISWABS > 0** and include reach numbers in record 5a (below)

3.3.2 Input format

For each simulation:

Read in subroutine STR1AL

1.	Data:	MXSTRM	NSS	NTRIB	NDIV	ICALC	CONST	ISTCB1	ISTCB2	ISWABS
	Format:	I10	I10	I10	I10	I10	F10.0	I10	I10	I10

For each stress period:

Read in subroutine STR1RP

2.	Data:	ITMP	IRDFLG	IPFLG
	Format:	I10	I10	I10

The following data set is read in sequential order of segment and reach.

3.	Data:	Layer	Row	Col	Seg	Reach	Flow	Stage	Cond	Sbot	Stop
	Format:	I5	I5	I5	I5	I5	F15.0	F10.0	F10.0	F10.0	F10.0

If stream stages for each reach are to be calculated (ICALC>0), then the following data set is read in sequential order of segment and reach.

4.	Data:	Width	Slope	Rough
	Format:	F10.0	F10.0	F10.0

If the maximum number of tributaries (NTRIB) that can join a segment is greater than zero, **and ISWABS≤0**, then the following data set is read. One record for each segment is read in sequential order. A record is necessary even for segments that do not have tributaries. In this case a blank record or a record with all zeros is read.

5. Data: Itrib(1) Itrib(2) ... Itrib(NTRIB)
 Format: I5 I5 ... I5

If the maximum number of tributaries (NTRIB) that can join a segment is greater than zero, **and ISWABS>0**, then the following data set is read. One record for each segment is read in sequential order. A record is necessary even for segments that do not have tributaries. In this case a blank record or a record with all zeros is read.

5a. Data: Inrch(1) Itrib(1) Inrch(2) Itrib(2) ... Inrch(NTRIB) Itrib(NTRIB)
 Format: I5 I5 I5 I5 ... I5 I5

If diversions are specified (NDIV>0), then the following data set is read. One record is read for each segment in sequential order. For segments that are not diversions, zeros or blanks are specified for each input item.

6. Data: lupseg
 Format: I10

3.3.3 Explanation of parameters used in input instructions

MXSTRM is the maximum number of stream reaches that can be active during the simulation.

NSS is the maximum number of segments that can be used during the simulation.

NTRIB is the maximum number of tributary segments that can join during a simulation. Ten is the maximum number allowed as currently specified in the program.

NDIV is a flag, which when positive, specifies that diversions from segments are to be simulated.

ICALC is a flag, which when positive, specifies that stream stages in reaches are to be calculated.

CONST is a constant value used in calculating stream stage in reaches. It is specified whenever ICALC is greater than zero. This constant is 1.486 for flow units of cubic feet per second and 1.0 for units of cubic meters per second. The constant must be multiplied by 86,400 when using time units of days in the simulation. (For an explanation of time units, see McDonald and Harbaugh, 1988, p. 4-10.)

ISTCB1 is a flag and a unit number.

If ISTCB1>0, it is the unit number to which leakage between each stream reach and the corresponding model cell will be saved on disk whenever the variable ICBCFL is specified. (See McDonald and Harbaugh, 1988, p. 4-15, for details about the Output Control Package used to specify ICBCFL.)

If ISTCB1=0, leakage between each reach and corresponding model cell will not be printed or filed on disk.

If ISTCB1<0, streamflows into and out of each reach and leakage between each reach and corresponding river cell will be printed whenever the variable ICBCFL is specified.

ISTCB2 is a flag and unit number for an option of storing accreted streamflow out of each reach instead of having the results printed.

If $ISTCB2 > 0$, it is the unit number where streamflow out of each reach will be saved on disk whenever the variable ICBCFL is specified.

If $ISTCB2 \leq 0$, streamflows out of each reach will not be saved on disk.

ISWABS is a flag.

If $ISWABS < 0$, surface water discharges and abstractions are allowed in ANY stream reach (abstraction rates are limited to the amount of flow available in the stream reach). Tributary inflows are only allowed in the first reach of a stream segment.

If $ISWABS = 0$, surface water discharges and tributary inflows are only allowed in the FIRST reach of a stream segment. Surface water abstractions are not allowed. This option allows the stream package to be used in the original way.

If $ISWABS > 0$, surface water discharges, abstractions and tributary inflows are allowed in ANY stream reach (abstraction rates are limited to the amount of flow available in the stream reach).

ITMP is a flag and a counter.

If $ITMP < 0$, stream data from the last stress period will be reused.

If $ITMP \geq 0$, ITMP will be the number of reaches active during the current stress period.

IRDFLG is a flag, which when positive, suppresses printing of the input data set specified for a stress period. The input data set is printed for a stress period if the value is zero or blank.

IPTFLG is a flag, which when positive, suppresses printing of results for a stress period. The results are printed for a stress period if the value is zero or blank and whenever the variable ICBCFL is specified.

Layer is the layer number of the cell containing the stream reach.

Row is the row number of the cell containing the stream reach.

Col is the column number of the cell containing the stream reach.

Seg is a number assigned to a group of reaches. Segments must be numbered in downstream order and are read into the program in sequential order.

Reach is a sequential number in a segment that begins with one for the farthest upstream reach and continues in downstream order to the last reach in the segment. Reaches must be read in sequentially as the order reaches are read into the program determines the order of connection of inflows and outflows.

Flow is the surface water abstraction/discharge or diversion flow [L^3T^{-1}] entering the segment.

If ISWABS=0, Flow is specified only for the first reach in each segment. The value is either a zero or a blank when the reach number (Reach) is not 1. When inflow into a segment is the sum of outflow from a specified number of tributary segments, the segment inflow values are specified as a -1.

If ISWABS<>0, Flow can be specified for any reach in any segment. Surface water abstractions can be simulated by entering a negative value (if the specified abstraction is greater than the available stream flow, all the flow is removed from the stream and a message is written to the output file detailing the reduction to the abstraction). Tributary inflows are handled entirely by the flow routing section in input block 5 (Itrib).

(Note: if the specified inflow to a diversion is greater than the flow in the reach from which flow is to be diverted, then no flow is diverted from the stream.)

Stage is the stream stage, in units of length.

Cond is the streambed hydraulic conductance, in units of length squared per time.

Sbot is the elevation of the bottom of the streambed, in units of length.

Stop is the elevation of the top of the streambed, in units of length.

Width is the width of the stream channel, in units of length. It is used only when the stream stage in each reach is to be calculated.

Slope is the slope of the stream channel in each reach, in units of length per length. It is used only when stream stage in each reach is calculated.

Rough is Mannings roughness coefficient for each stream reach. It is used only when stream stage in each reach is calculated.

Itrib(1) for a segment that has tributary segments, Itrib(1) is the number of the first tributary segment. For a segment with no tributaries, Itrib(1) must be specified as zero.

Itrib(2) for a segment that has tributary segments, Itrib(2) is the number of the second tributary segment. For a segment with no or only one tributary segment, Itrib(2) must be specified as zero.

Inrch(1) for a segment that has tributary segments, if tributaries are allowed in any stream reach (ISWABS>0), Inrch(1) is the number of the reach that the first tributary flows into.

Inrch(2) for a segment that has tributary segments, if tributaries are allowed in any stream reach (ISWABS>0), Inrch(2) is the number of the reach that the second tributary flows into.

lupseg for a diversion segment, lupseg is the number of the upstream segment from which water is diverted. For a segment that is not a diversion, lupseg must be specified as zero.

3.3.4 Example stream input file

	150	12	2	0	0	86400	50	51	
	150	0	0	Inflow	Stage	Cond.	Bottom	Top	
1	54	57	1	1	10	85.28	2.50E+04	84.28	85.28
1	55	57	1	2	10	85.217	2.50E+04	84.217	85.217
1	55	56	1	3	10	84.43	2.50E+04	83.43	84.43
1	55	55	1	4	10	83.303	2.50E+04	82.303	83.303
1	56	55	1	5	10	82.579	2.50E+04	81.579	82.579
1	56	54	1	6	10	81.629	2.50E+04	80.629	81.629
1	56	54	1	7	10	80.683	2.50E+04	79.683	80.683
1	56	54	1	8	10	79.737	2.50E+04	78.737	79.737
1	60	52	1	11	10	74.752	2.50E+04	73.752	74.752
1	61	52	1	12	10	73.204	2.50E+04	72.204	73.204
1	62	51	1	13	10	71.734	2.50E+04	70.734	71.734
1	63	51	1	14	10	69.944	2.50E+04	68.944	69.944
1	64	51	1	15	10	68.695	2.50E+04	67.695	68.695
1	65	51	1	16	10	67.446	2.50E+04	66.446	67.446
1	66	51	1	17	10	66.411	2.50E+04	65.411	66.411
1	66	52	1	18	10	63.489	2.50E+04	62.489	63.489
1	67	52	1	19	10	64.192	2.50E+04	63.192	64.192
1	68	52	1	20	10	61.216	2.50E+04	60.216	61.216
1	69	52	1	21	10	58.591	2.50E+04	57.591	58.591
1	70	52	1	22	10	56.655	2.50E+04	55.655	56.655
1	67	54	1	23	10	68.455	2.50E+04	67.455	68.455
1	68	54	1	24	10	65.457	2.50E+04	64.457	65.457
1	70	61	1	25	10	77.85	2.50E+04	76.85	77.85
1	70	60	1	26	10	76.425	2.50E+04	75.425	76.425
1	70	59	1	27	10	72.874	2.50E+04	71.874	72.874
1	69	58	1	28	10	69.82	2.50E+04	68.82	69.82
1	68	57	1	29	10	68.802	2.50E+04	67.802	68.802
1	68	56	1	30	10	66.901	2.50E+04	65.901	66.901
1	69	57	1	31	10	66.837	2.50E+04	65.837	66.837
1	69	56	1	32	10	65.173	2.50E+04	64.173	65.173
1	69	55	1	33	10	63	2.50E+01	62	64
1	69	54	1	34	10	61.23	2.50E+04	60.23	61.23
1	80	56	1	35	10	70.348	2.50E+04	69.348	70.348
1	79	56	8	2	10	70.757	2.50E+04	69.757	70.757
1	78	56	8	3	10	69.716	2.50E+04	68.716	69.716
1	78	55	8	4	10	68.756	2.50E+04	67.756	68.756
1	77	55	8	5	10	67.646	2.50E+04	66.646	67.646
								668	
								278	
								272	
								277	
1	72	55	8	10	10	59.745	2.50E+04	58.745	59.745
1	71	53	8	11	10	58.342	2.50E+04	57.342	58.342
1	70	53	8	12	10	57.321	2.50E+04	56.321	57.321
1	71	52	8	13	10	55.535	2.50E+04	54.535	55.535
1	71	51	8	14	10	55.01	2.50E+04	54.01	55.01
1	70	50	8	15	10	53.936	2.50E+04	52.936	53.936
1	70	49	8	16	10	52.932	2.50E+04	51.932	52.932
1	70	48	8	17	10	51.936	2.50E+04	50.936	51.936
1	69	48	8	18	10	51.191	2.50E+04	50.191	51.191
1	69	47	8	19	10	50.218	2.50E+04	49.218	50.218
1	69	46	8	20	10	49.244	2.50E+04	48.244	49.244
1	69	45	8	21	10	48.307	2.50E+04	47.307	48.307
1	69	44	8	22	10	47.542	2.50E+04	46.542	47.542
1	70	44	8	23	10	47.029	2.50E+04	46.029	47.029
1	70	43	8	24	10	46.361	2.50E+04	45.361	46.361
1	69	42	8	25	10	45.454	2.50E+04	44.454	45.454
1	69	41	8	26	10	45.164	2.50E+04	44.164	45.164
1	70	40	8	27	10	43.82	2.50E+04	42.82	43.82
1	69	39	8	28	10	42.498	2.50E+04	41.498	42.498
1	70	38	8	29	10	41.332	2.50E+04	40.332	41.332
1	71	37	8	30	10	40.361	2.50E+04	39.361	40.361
1	54	45	9	1	10	75.623	2.50E+04	74.623	75.623
1	54	44	9	2	10	74.618	2.50E+04	73.618	74.618
1	54	43	9	3	10	73.693	2.50E+04	72.693	73.693
1	55	43	9	4	10	72.586	2.50E+04	71.586	72.586
1	55	42	9	5	10	71.371	2.50E+04	70.371	71.371
1	55	41	9	6	10	74.932	2.50E+04	73.932	74.932
1	56	41	9	7	10	73.817	2.50E+04	72.817	73.817
1	56	40	9	8	10	72.491	2.50E+04	71.491	72.491
1	56	39	9	9	10	71.417	2.50E+04	70.417	71.417
1	56	38	9	10	10	69.297	2.50E+04	68.297	69.297
1	56	37	9	11	10	67.58	2.50E+04	66.58	67.58
1	56	36	9	12	10	66.361	2.50E+04	65.361	66.361
1	55	36	9	13	10	65.224	2.50E+04	64.224	65.224
1	55	35	9	14	10	64.419	2.50E+04	63.419	64.419

Item: 2
Variables: ITMP, IRDFLG & IPTFLG

Item: 1
Variable: ISWABS
Value: 1
Option: **Surface water discharges, abstraction & tributary inflows allowed in any stream reach.**

Item: 3
Variable: Flow
Value: 10
Option: **Flow of 10 m³/d added to each stream reach (can be used to represent inflow from surface water runoff).**

Item: 3
Variables: Layer, Row, Col, Seg, Reach, Flow, Stage, Cond, Sbot, Stop

1	55	34	9	15	10	62.809	2.50E+04	61.809	62.809
1	55	33	9	16	10	61.502	2.50E+04	60.502	61.502
1	55	32	9	17	10	59.619	2.50E+04	58.619	59.619
1	54	32	9	18	10	58.363	2.50E+04	57.363	58.363
1	53	32	9	19	10	56.553	2.50E+04	55.553	56.553
1	52	31	9	20	10	55.778	2.50E+04	54.778	55.778
1	52	30	9	21	10	55.522	2.50E+04	54.522	55.522
1	52	29	9	22	10	55.011	2.50E+04	54.011	55.011
1	52	28	9	23	10	54.467	2.50E+04	53.467	54.467
1	51	28	9	24	10	53.964	2.50E+04	52.964	53.964
1	51	27	9	25	10	53.515	2.50E+04	52.515	53.515
1	51	26	9	26	10	53.004	2.50E+04	52.004	53.004
1	51	25	9	27	10	52.524	2.50E+04	51.524	52.524
1	50	25	9	28	10	52.066	2.50E+04	51.066	52.066
1	50	24	9	29	10	51.599	2.50E+04	50.599	51.599
1	50	23	9	30	10	51.172	2.50E+04	50.172	51.172
1	51	22	9	31	10	51	5.00E+01	50	51
1	35	45	12	1	10	88.321	2.50E+04	87.321	88.321
1	34	44	12	2	10	86.553	2.50E+04	85.553	86.553
1	34	43	12	3	10	85.111	2.50E+04	84.111	85.111
1	34	42	12	4	10	83.88	2.50E+04	82.88	83.88
1	35	42	12	5	10	82.542	2.50E+04	81.542	82.542
1	35	41	12	6	10	81.443	2.50E+04	80.443	81.443
1	35	40	12	7	10	80.296	2.50E+04	79.296	80.296
1	35	39	12	8	10	79.594	2.50E+04	78.594	79.594
1	36	39	12	9	10	78.481	2.50E+04	77.481	78.481
1	36	38	12	10	10	77.524	2.50E+04	76.524	77.524
1	37	38	12	11	10	76.53	2.50E+04	75.53	76.53
1	37	37	12	12	10	75.219	2.50E+04	74.219	75.219
1	37	36	12	13	10	73.817	2.50E+04	72.817	73.817
1	37	35	12	14	10	72.559	2.50E+04	71.559	72.559
1	38	35	12	15	10	71.19	2.50E+04	70.19	71.19
1	38	34	12	16	10	69.88	2.50E+04	68.88	69.88
1	39	34	12	17	10	69.082	2.50E+04	68.082	69.082
1	39	33	12	18	10	67.985	2.50E+04	66.985	67.985
1	38	32	12	19	10	65.571	2.50E+04	64.571	65.571
1	38	31	12	20	10	64.485	2.50E+04	63.485	64.485
1	39	31	12	21	10	63.257	2.50E+04	62.257	63.257
1	40	31	12	22	10	61.971	2.50E+04	60.971	61.971
1	40	30	12	23	10	61.204	2.50E+04	60.204	61.204
1	41	30	12	24	10	60.668	2.50E+04	59.668	60.668
1	41	29	12	25	10	60.329	2.50E+04	59.329	60.329
1	41	28	12	26	10	59.594	2.50E+04	58.594	59.594
1	42	28	12	27	10	58.9	2.50E+04	57.9	58.9
1	43	28	12	28	10	58.22	2.50E+04	57.22	58.22
1	44	28	12	29	10	57.561	2.50E+04	56.561	57.561
1	45	28	12	30	10	56.942	2.50E+04	55.942	56.942
1	45	27	12	31	10	56.394	2.50E+04	55.394	56.394
1	45	26	12	32	10	55.669	2.50E+04	54.669	55.669
1	46	26	12	33	10	54.912	2.50E+04	53.912	54.912
1	46	25	12	34	10	54.167	2.50E+04	53.167	54.167
1	46	24	12	35	10	53.527	2.50E+04	52.527	53.527
1	46	23	12	36	10	52.971	2.50E+04	51.971	52.971
1	46	22	12	37	10	52.336	2.50E+04	51.336	52.336
1	46	21	12	38	10	51.741	2.50E+04	50.741	51.741
1	46	20	12	39	10	51.199	2.50E+04	50.199	51.199
1	46	19	12	40	10	50.592	2.50E+04	49.592	50.592
1	46	18	12	41	10	49.395	2.50E+04	48.395	49.395
1	46	17	12	42	10	48.55	2.50E+04	47.55	48.55
1	46	16	12	43	10	47.66	2.50E+04	46.66	47.66
1	46	15	12	44	10	46.832	2.50E+04	45.832	46.832
1	46	14	12	45	10	46.203	2.50E+04	45.203	46.203
1	52	18	12	46	10	45.552	2.50E+04	44.552	45.552
1	52	17	12	47	10	44.972	2.50E+04	43.972	44.972
1	53	17	12	48	10	44.063	2.50E+04	43.063	44.063
1	53	16	12	49	10	43.12	2.50E+04	42.12	43.12
1	54	16	12	50	10	42.047	2.50E+04	41.047	42.047
1	55	16	12	51	10	41.245	2.50E+04	40.245	41.245
1	55	15	12	52	10	40.733	2.50E+04	39.733	40.733
1	56	15	12	53	10	40.494	2.50E+04	39.494	40.494
1	57	15	12	54	10	40.022	2.50E+04	39.022	40.022
1	57	14	12	55	10	39.558	2.50E+04	38.558	39.558
0	0	0	0	0	10				
0	0	0	0	0	10				
0	0	0	0	0	10				
10	3	0	0	0	10				
0	0	0	0	0	10				
0	0	0	0	0	10				
13	1	12	4	0	10				
0	0	0	0	0	10				
0	0	0	0	0	10				
43	9	0	0	0	10				
-1	-1	1	0	0	10				
-1	-1	1	0	0	10				
-1	-1	1	0	0	10				

Item: 3
 Variable: Flow
 Value: -50,000
 Option: Flow of 50,000 m³/d
 taken from stream reach
 (can be used to represent
 surface water abstraction).

Item: 5a
 Variables: Inrch(1), Itrib(1),...
 Values: 10, 3,...
 Option: Stream segment 3 is a
 tributary flowing into
 reach 10 of segment 4.

Item: 5a

Item: 2
 Variables: ITMP, IRDFLG
 & IPTFLG
 (Data repeated for stress
 periods 2-4)

3.4 Module documentation for stream package

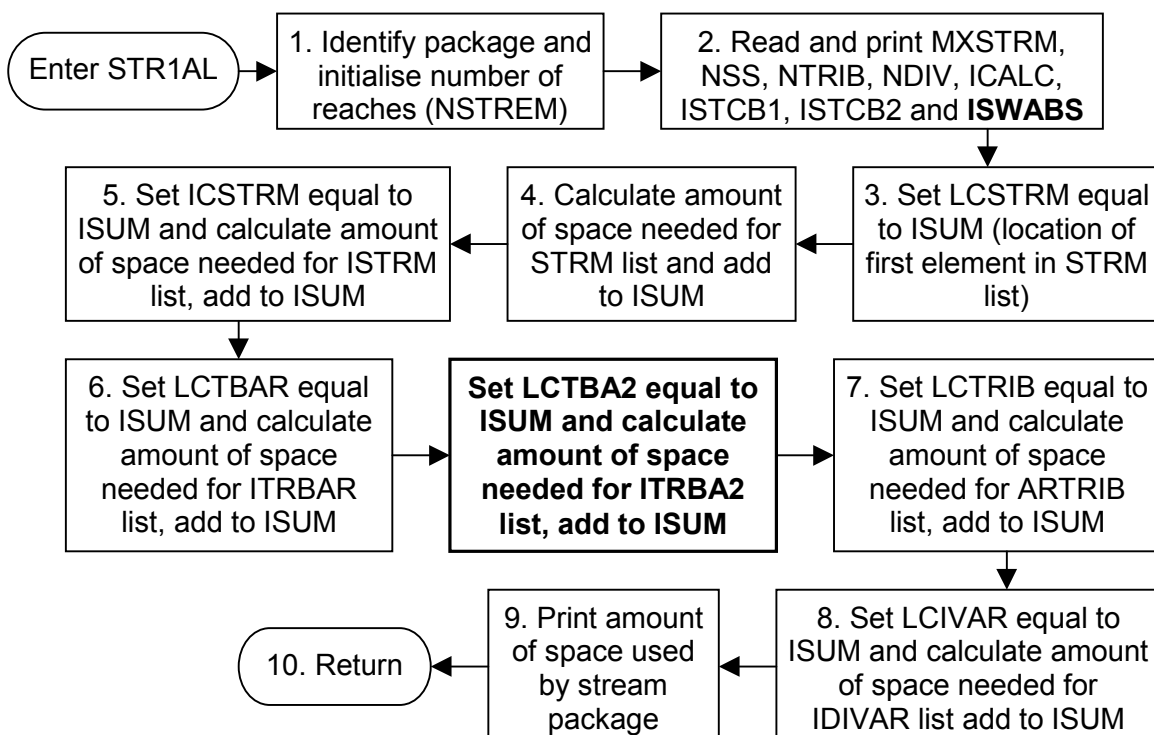
Modifications have been made to all four of the original modules of the stream routing package (STR-VKD1). No extra modules have been added. All of the modules are called by the MAIN program. The modules are:

- STR1AL Allocates space for arrays used in the package.
 STR1RP Reads all data needed by the package and initialises reach inflow, outflow, and leakage arrays.
 STR1FM Calculates leakage to and from stream reaches and adds appropriate terms to finite-difference equations used to calculate heads in aquifer and simulate groundwater flow.
 STR1BD Calculates rates and accumulated volumes of stream leakage into and out of aquifer. Results are either saved on files or printed.

3.4.1 Changes to module STR1AL

- Different title printed to listing file
- Read in new input flag (ISWABS - activates new options)
- Print message to output file if new options are activated
- Allocate storage space for new array (ITRBA2 – holds extra tributary routing info)

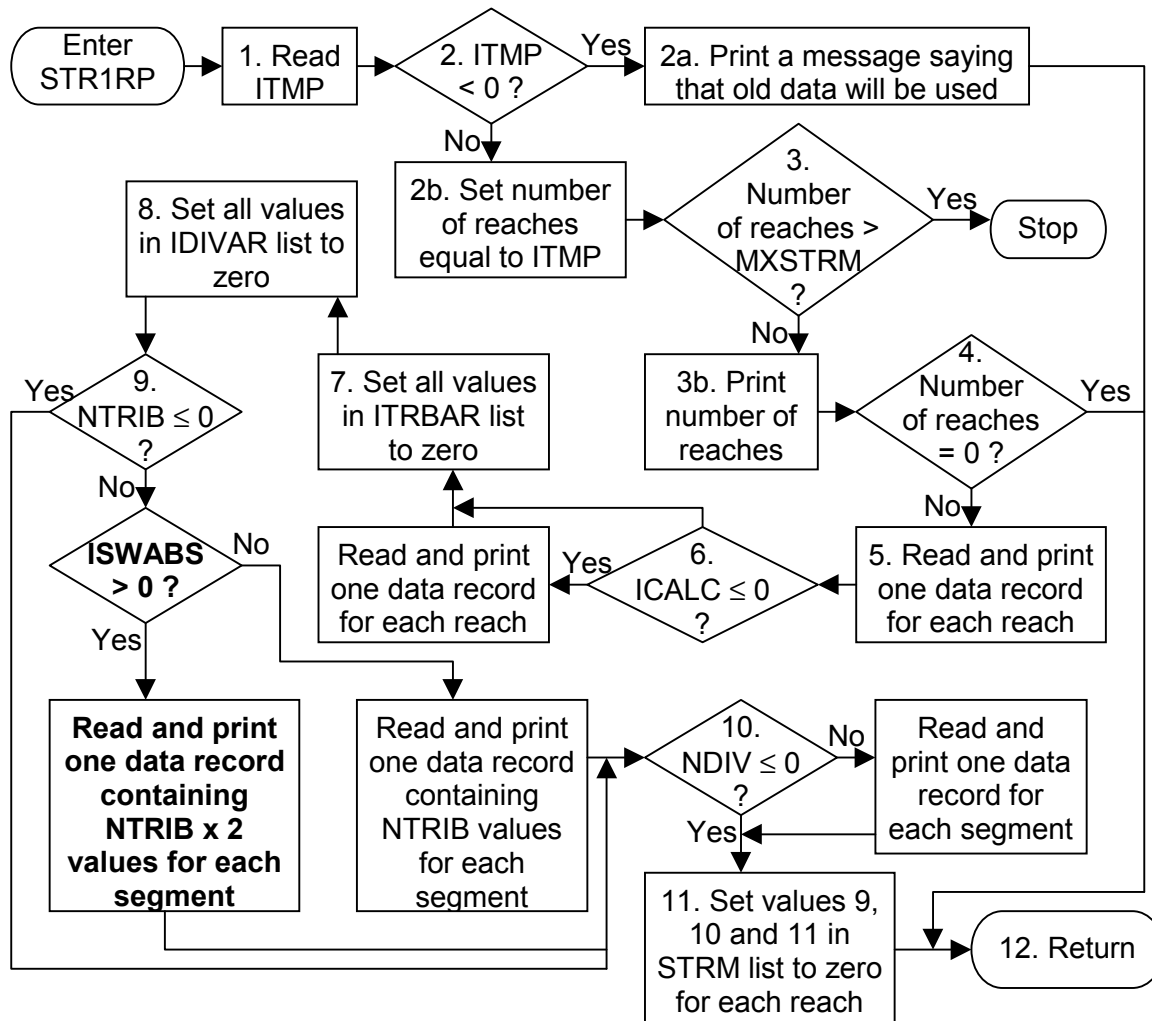
Flow Chart for module STR1AL



3.4.2 Changes to module STR1RP

- Dimension new array ITRBA2
- Change input format if ISWABS is greater than zero
- Change format of input echoed to listing file

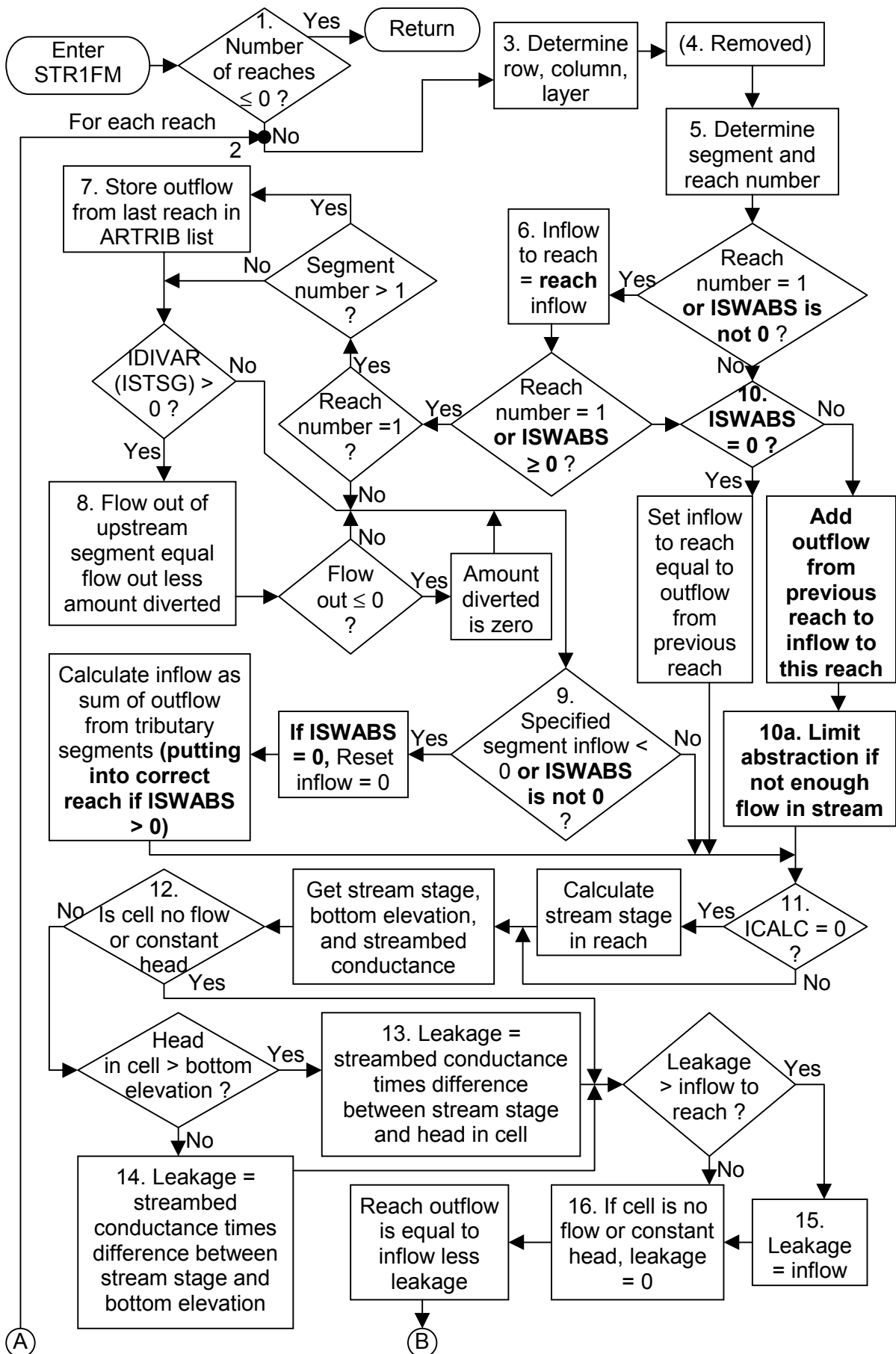
Flow chart for module STR1RP

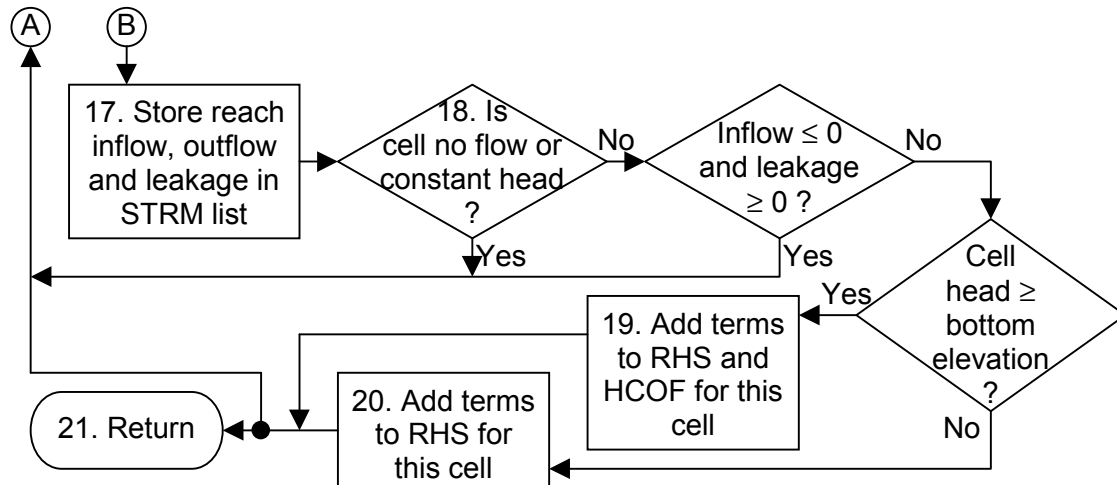


3.4.3 Changes made to STR1FM

- Dimension new array ITRBA2.
- Allow surface water abstraction or discharge if ISWABS is not zero.
- Allow tributary inflows at any reach in a segment if ISWABS is greater than zero.
- Limit surface water abstraction if there is not enough flow available in the stream.

Flow chart for module STR1FM

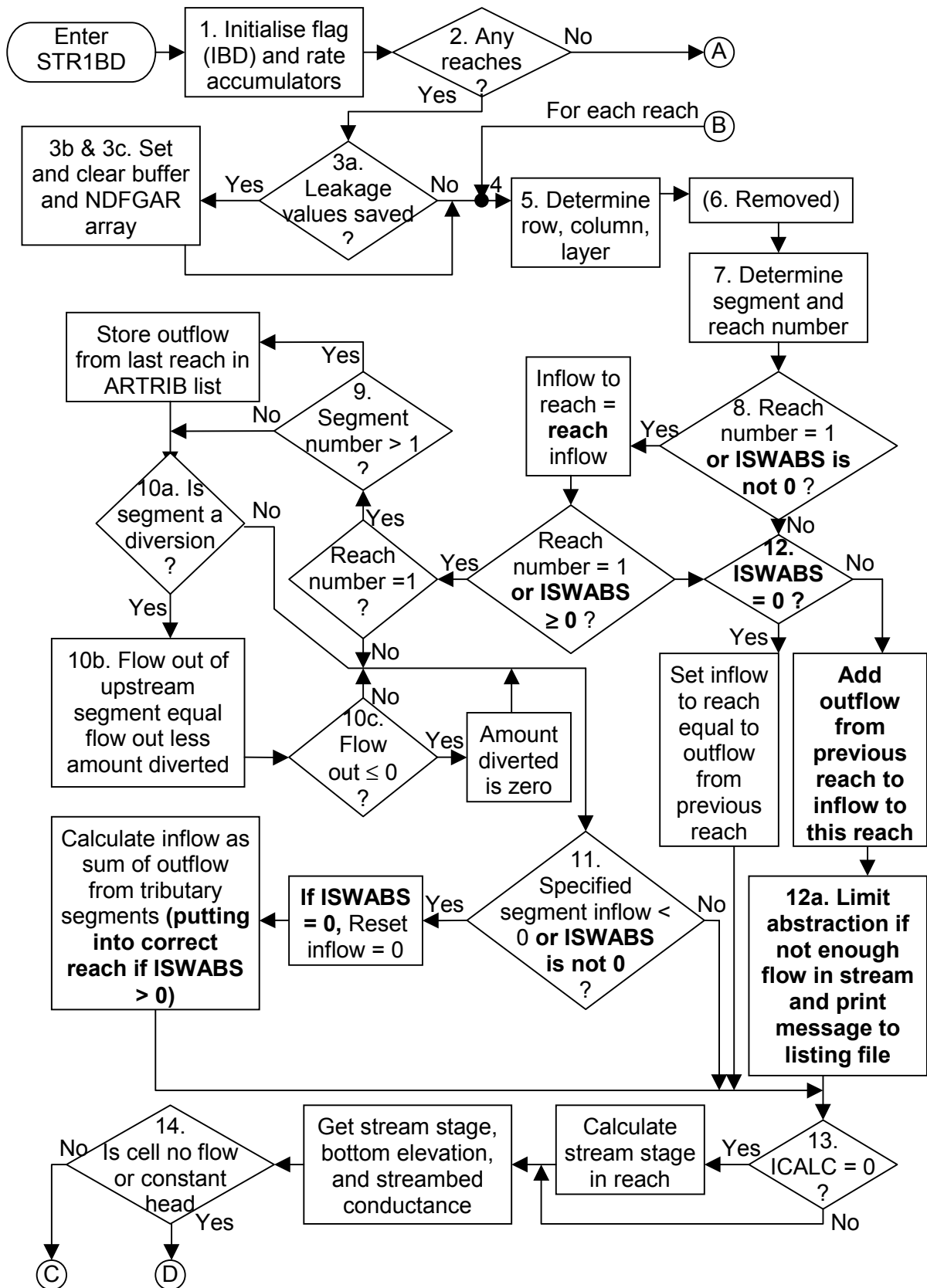


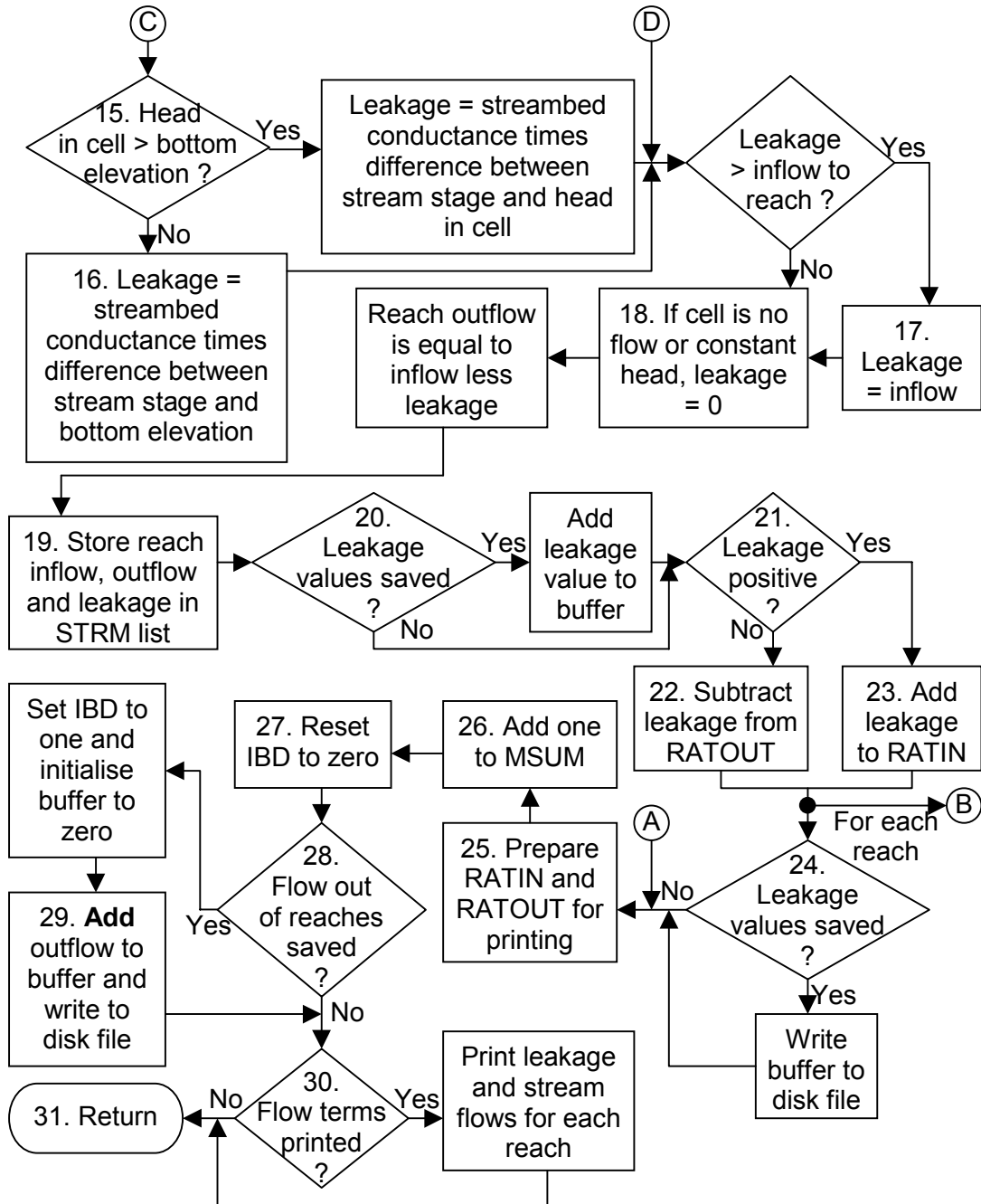


3.4.4 Changes made to STR1BD

- Dimension new array ITRBA2
- Allow surface water abstraction or discharge if ISWABS is not zero
- Allow tributary inflows at any reach in a segment if ISWABS is greater than zero
- Limit surface water abstraction if there is not enough flow available in the stream and print a message to the listing file

Flow chart for module STR1BD





4 PRECONDITIONED CONJUGATE-GRADIENT SOLVER PACKAGE

4.1 Introduction

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

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

4.2 New features included

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

4.2.1 Progress monitor

The first modification prints convergence information to the screen whilst the model is running so that the progress of the simulation can be monitored. An input flag does not control this modification; the progress monitor will always be displayed when the PCG solver is used. The information written to the screen includes the stress period, the time step, the iteration and the current degree of convergence in terms of the head difference and the flow residual.

4.2.2 Force convergence if criteria met for a specified number of iterations

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

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

4.2.3 Debugging option

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

Position in file (bytes)	Data in heads file	Data in debug file	Data type
0	Time step	Inner iteration	Integer
4	Stress period	Outer iteration	Integer
8	Stress period time	Largest head difference	Real
12	Total time	Largest residual	Real
16	"HEAD"	"Unconverged Head"	Text
32	Number of columns	Number of columns	Integer
36	Number of rows	Number of rows	Integer
40	Layer number	Layer number	Integer
44	Head values	Unconverged head values	Real array

4.3 Input instructions

4.3.1 Summary of new options

This new version of the MODFLOW modelling code allows three new options to be set (shown in **bold**) in the input instructions for the PCG package. The new code should still be compatible with old MODFLOW input files (versions up to MODFLOW-96). The new options included are:

- **Progress monitor** - automatically runs when using PCG solver
- **Force convergence if criteria met for specified number of outer iterations** - set **NOUTC > 0**
- **Debugging option** - set IPCGDEBUG > 0 and specify a file name in the NAME file

4.3.2 Input format

For each simulation:

Read in subroutine PCG2AL

1.	Data:	MXITER	ITER1	NPCOND	NOUTC	IPCGDEBUG
	Format:	I10	I10	I10	I10	I10

Read in subroutine PCG2RP

2.	Data:	HCLOSE	RCLOSE	RELAX	NBPOL	IPRPCG	MUTPCG	DAMP
	Format:	F10.0	F10.0	F10.0	I10	I10	I10	F10.0

4.3.3 Explanation of parameters used in input instructions

MXITER is the maximum number of outer iterations – that is, calls to the solution routine. For a linear problem MXITER should be 1, unless more than 50 inner iterations are required, when MXITER could be as large as 10. A larger number (generally less than 100) is required for a nonlinear problem.

ITER1 is the maximum number of inner iterations. For nonlinear problems, ITER1 usually ranges from 3 to 10; a value of 30 will be sufficient for most linear problems.

NPCOND is the flag used to select the matrix preconditioning method. The following options are available.

NPCOND	Preconditioning method
1	Modified Incomplete Cholesky (for use on scalar computers (PCs))
2	Polynomial (for use on vector computers or to conserve computer storage)

NOUTC is the maximum number of consecutive outer iterations during which the criteria are met before convergence is ‘forced’ (can lead to invalid results). If NOUTC is 0 then convergence will not be forced.

IPCGDEBUG is a flag and a unit number.

If IPCGDEBUG > 0, it is the unit number on which unconverged head values will be recorded. A record is written every iteration, and is cleared each time a time step converges. This option slows the simulation down as output is written every iteration. The size of the file will be large if a large number of iterations are allowed.

If IPCGDEBUG = 0, unconverged head values will not be recorded.

HCLOSE is the head change criterion for convergence, in units of length. When the maximum absolute value of the head change at all nodes during an iteration is less than or equal to HCLOSE, and the criterion for RCLOSE is satisfied (see below), iteration stops.

RCLOSE is the residual criterion for convergence, in units of cubic length per time. When the maximum absolute value of the residual at all nodes during an iteration is less than or equal to RCLOSE, and the criterion for HCLOSE is satisfied (see above), iteration stops.

For nonlinear problems, convergence is achieved when the convergence criteria are satisfied on the first inner iteration.

RELAX is the relaxation parameter used with NPCOND=1 (MICCG). Usually, RELAX=1.0, but for some problems a value of 0.99 or 0.97 will reduce the number of iterations required for convergence. RELAX is not used if NPCOND is not 1.

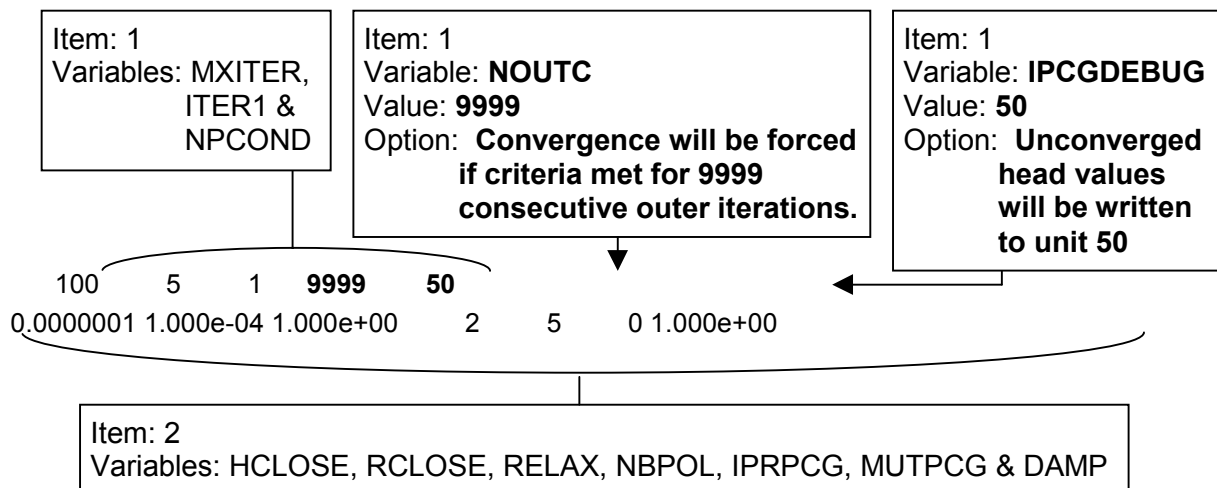
NBPOL is used when NPCOND=2 to indicate whether the estimate of the upper bound on the maximum eigenvalue is 2.0, or whether the estimate will be calculated. NBPOL=2 is used to specify the value as 2.0; for any other value of NBPOL, the estimate is calculated. Convergence is generally insensitive to this parameter. NBPOL is not used if NPCOND does not equal 2.

IPRPCG is the printout interval for PCG. If IPRPCG is equal to zero, it is changed to 999. The extreme head change and residual (positive or negative) are printed for each iteration of a time step whenever the time step is an even multiple of IPRPCG. The printout also occurs at the end of each stress period regardless of the value of IPRPCG.

MUTPCG is a flag which controls printing from the solver. If MUTPCG is not 0, printing from the solver is suppressed. If MUTPCG=1, the number of iterations is printed, but the lists of extreme head changes and residuals is suppressed. If MUTPCG=2, all printing is suppressed.

DAMP is the damping parameter. DAMP can be used to reduce oscillation when the solver is having difficulty converging due to excessive oscillation. The value of DAMP is a multiplier for the head change calculated each iteration at all cells. Thus, if DAMP is 0.5, the head change is cut in half. If DAMP is 1.0, then PCG2 behaves as it did prior to the addition of this capability. DAMP should be set equal to 1.0 except when there is indication of excessive oscillation. If the value of DAMP is specified as 0.0 or less, it is automatically changed to 1.0.

4.3.4 Example PCG input file



4.4 Module documentation for PCG package

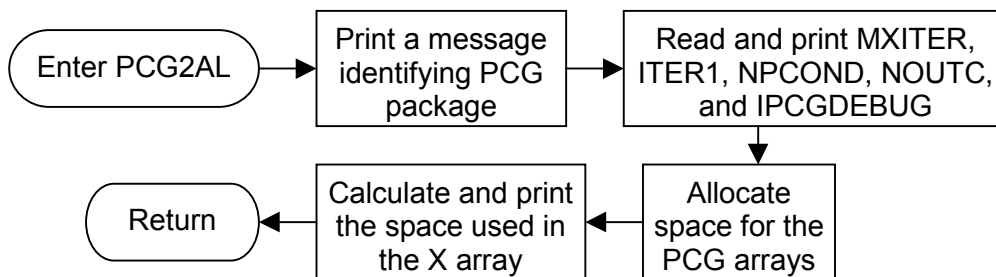
The modified Preconditioned Conjugate Gradient package (PCG-VKD1) has had changes made to two of the three primary modules. These modules are:

PCG2AL Allocates space for arrays used in the package & reads new input parameters
 PCG2RP Reads remaining input parameters – not changed
 PCG2AP Solves the groundwater flow equations

4.4.1 Changes to module PCG2AL

- Changed title printed to listing file
- Read in new input parameters and write options to listing file

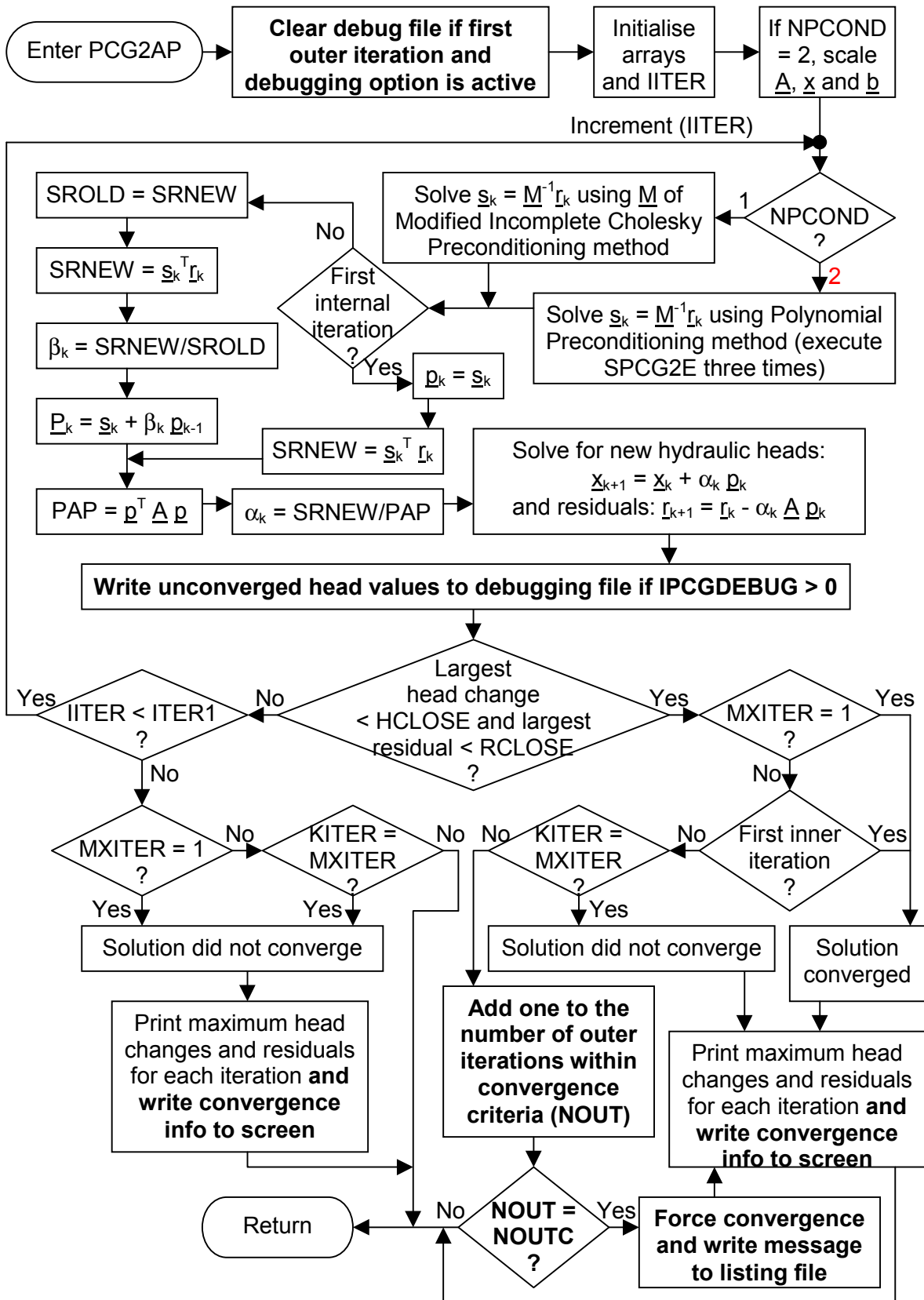
Flow chart for module PCG2AL



4.4.2 Changes to module PCG2AP

- Write unconverged head values to debugging file if IPCGDEBUG > 0
- Force convergence if NOUTC outer iterations are within the convergence criteria and write warning to listing file
- Write convergence information to the screen

Flow chart for module PCG2AP



5 MODFLOW UTILITIES PACKAGE

5.1 Introduction

The utilities package contains routines to read data from and write data to data files. Its main functions include reading one and two dimensional real and integer arrays, and writing arrays to the output file or to binary files. A description of the array input formats is included here for completeness (the BCF package uses the array readers). This is followed by a description of the modifications to allow the use of direct access binary files.

5.2 Array input

The routines for reading arrays have not been modified. The input format for array inputs is reproduced here for completeness. For more details see Harbaugh & McDonald, 1996.

The real two-dimensional array reader (U2DREL), the integer two-dimensional array reader (U2DINT), and the real one-dimensional array reader (U1DREL) read one array-control record and, optionally, a data array in a format specified on the array control record. The control record is read from the input unit number specified for the major option that is requesting the array. For example, the Recharge Package uses U2DREL to read the RECH array. The input unit for the recharge option is contained in IUNIT (8), and accordingly, the RECH array control record is read on this input unit.

For real array reader (U2DREL or U1DREL)

Data:	LOCAT	CNSTNT	FMTIN	IPRN
Format:	I10	F10.0	5A4	I10

For integer array reader (U2DINT)

Data:	LOCAT	ICONST	FMTIN	IPRN
Format:	I10	I10	5A4	I10

5.2.1 Explanation of fields used in input instructions

LOCAT indicates the location of the data which will be put in the array.

If LOCAT < 0, the sign is reversed to give the unit number from which an unformatted record will be read.

If LOCAT = 0, every element in the array will be set equal to the value CNSTNT or ICONST.

If LOCAT > 0, it is the unit number from which data values will be read in the format specified in the third field of the array-control record (FMTIN).

CNSTNT/ICONST is a constant. Its use depends on the value of LOCAT.

If LOCAT = 0, every element in the array is set equal to CNSTNT/ICONST.

If LOCAT is not 0, and if CNSTNT/ICONST is not 0, every element in the array is multiplied by CNSTNT/ICONST.

FMTIN is the format of records containing the array values. It is used only if the first field in the array-control record (LOCAT) contains a positive number. The format must be enclosed in parentheses; for example, (15F5.0) for real data and (15I5) for integer data. The format must be either a standard Fortran format, "(FREE)" which indicates free format, or "(BINARY)" which indicates binary (unformatted) data. When using a free-format control record, the format must be enclosed in apostrophes if it contains one or more blanks or commas. There are only 2 ways to create a binary file that can be read by MODFLOW. The first way is to use MODFLOW to create the file by saving heads in a binary file (but not a direct access binary file – see Section 5.3.1). This is commonly done when it is desired to use computed heads from one simulation as initial heads for a subsequent simulation. The other way to create a binary file is to write a special program that generates a binary file. "(FREE)" and "(BINARY)" can only be specified in free-format control records (see below). Also, "(BINARY)" can only be specified when using U2DREL or U2DINT, and only when the control record is EXTERNAL or OPEN/CLOSE. When the "(FREE)" option is used, be sure that all array elements have a non-blank value and that a comma or at least one blank separates adjacent values.

IPRN is a flag indicating that the array being read should be printed and a code for indicating the format that should be used. It is used only if LOCAT is not equal to zero. The format codes are different for each of the three modules. IPRN is set to zero when the specified value exceeds those defined in the chart below. If IPRN is less than zero, the array will not be printed.

IPRN	U2DREL	U2DINT	U1DREL
0	10G11.4	10I11	10G12.5
1	11G10.3	60I1	
2	9G13.6	40I2	
3	15F7.1	30I3	
4	15F7.2	25I4	
5	15F7.3	20I5	
6	15F7.4		
7	20F5.0		
8	20F5.1		
9	20F5.2		
10	20F5.3		
11	20F5.4		
12	10G11.4		

5.2.2 Free-format control records for array readers

In addition to the fixed format control records described above, free-format can also be used. Values in italics are key words that can be specified as uppercase or lowercase. Each control record is limited to a length of 79 characters.

1. *CONSTANT* *CNSTNT*

All values in the array are set equal to *CNSTNT*.

2. *INTERNAL* *CNSTNT* *FMTIN* *IPRN*

The individual array elements will be read from the same file that contains the control record.

3. *EXTERNAL* *Nunit* *CNSTNT* *FMTIN* *IPRN*

The individual array elements will be read from the file unit number specified by *Nunit*. The name of the file associated with this file unit must be contained in the name file.

4. *OPEN/CLOSE* *FNAME* *CNSTNT* *FMTIN* *IPRN*

The array will be read from the file whose name is specified by *FNAME*. This file will be opened on unit 99 just prior to reading the array and closed immediately after the array is read. This file should not be included in the name file. A file that is read using this control record can contain only a single array. The *OPEN/CLOSE* option is particularly useful for running simulations that require more than 99 files using a computer that allows only 99 files to be opened simultaneously.

5.3 New features

The only change made to the utilities package was to allow the use of direct access binary output files.

5.3.1 Allow use of direct access binary files

The routine in the Basic package that opens all the files in the NAME file (SBAS50) allows the user to specify a binary file as a direct access file by entering the word 'DIRECT' after the filename. A number specifying the record length of the direct access file (in bytes) should follow this keyword (a value of 1 will ensure that the file opens without an error – see Section 6.2 for details).

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

Note: This option works with code compiled using the Salford FTN77 compiler; it does not work using the Compaq Fortran compiler.

5.4 Module documentation for utilities package

The modified Utility package (UTL-VKD1) has had changes made to two of the modules. These modules are:

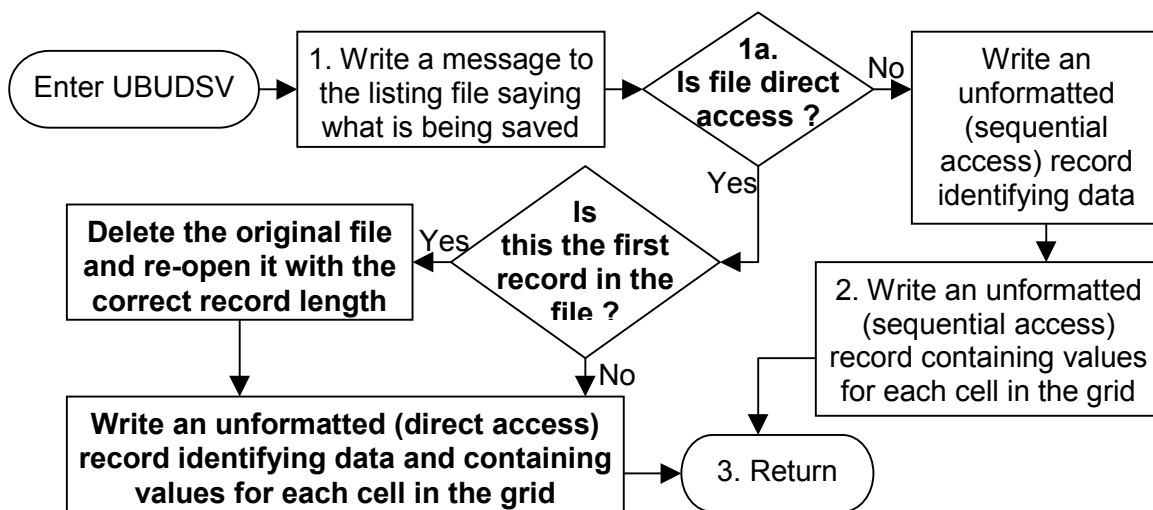
UBUDSV Records cell-by-cell flow terms for one component of flow

ULASAV Saves a one-layer array on disk (used for head and drawdown output)

5.4.1 Changes to module UBUDSV

- Allow use of direct access binary files

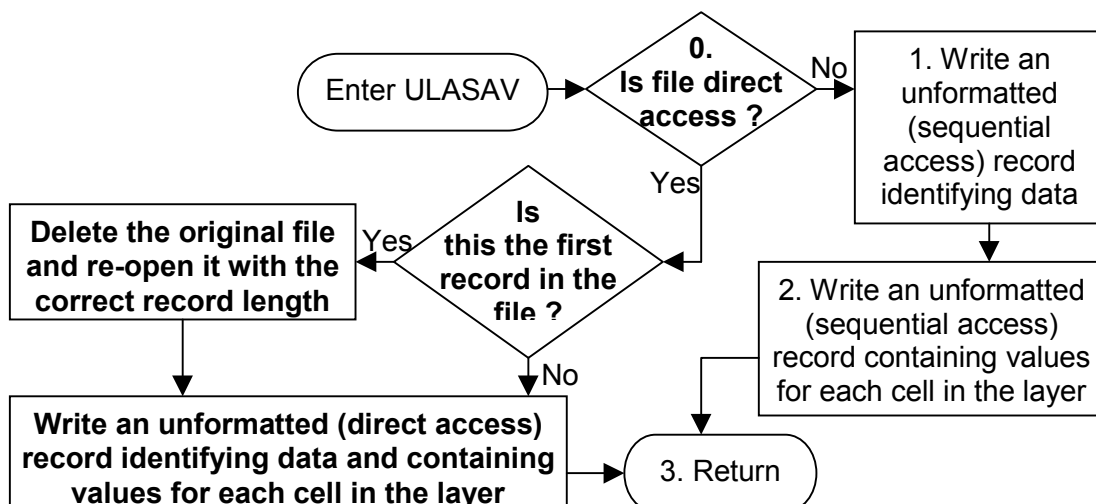
Flow chart for module UBUDSV



5.4.2 Changes to module ULASAV

- Allow use of direct access binary files

Flow chart for module ULASAV



6 MAIN PROGRAM

6.1 Description of changes to main program

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

- Increased the size of the X array from 1,500,000 to 10,000,000. (This allows the code to use a maximum of 38 MB of memory, however, many operating systems use dynamic storage meaning that the memory requirements will depend on the size of the model being simulated.)
- Allow the progress monitor to be printed to the screen when using the PCG solver (see Section 4.2.1).
- Allow the code to loop back and run a second simulation when using the auto conversion option (see Section 2.2.3).
- Allow the output of calculated transmissivity values to the listing file (see Section 2.2.7).
- Change all the 'real' variables to 'double precision' variables. This allows for the greater precision required for the calculation of variations in storage with depth.

6.2 Input instructions for the name file

The name file is a special file that is read by the Basic Package. The name file is read on unit 99, as specified in the MAIN program. The name file must specify the names of all files being used in a model simulation except for OPEN/CLOSE files (see Section 6.2.1). As a minimum, there must be a listing file to which all model output intended for printing will be written and one input file for each package being used. (Output that goes to the listing file is frequently referred to as printed output because it is expected that all or parts of this file will be printed.) There may also be additional input files containing array data and output files for saving head, drawdown, and cell-by-cell budget data.

This new version of the MODFLOW modelling code allows some new options to be set (shown in **bold**) in the name file.

For each simulation

1. Ftype Nunit Fname [*DIRECT* Recl] [**> Fname2 [*DIRECT* Recl]]**

The name file must contain one of the above records (item 1) for each file used in the simulation. The first record must be for the listing file; the remaining records can be in any order. All parameters are free format. The length of each record must be 79 characters or less. The items in square brackets are optional.

Any number of comment records, which are indicated by the # character in column one, can be interspersed among the item-1 records. Any text characters can follow the # character. Comment records have no effect on the simulation; their purpose is to allow users to provide documentation about a particular simulation. All comment records that come after the first item-1 record are written in the listing file.

6.2.1 Explanation of parameters in the name file

Ftype is the file type, which must be one of the following character values. Ftype may be entered in uppercase or lowercase:

LIST for the listing file (main output file)
 BAS for the Basic Package
 BCF for the Block Centred Flow Package
 WEL for the Well Package
 DRN for the Drain Package
 RIV for the River Package
 EVT for the Evapotranspiration Package
 TLK for the Transient Leakage Package
 GHB for the General Head Boundary Package
 RCH for the Recharge Package
 SIP for the Strongly Implicit Procedure (solver) Package
 DE4 for the D4 Direct Solution (solver) Package
 SOR for the Slice Successive Over Relaxation (solver) Package
 OC for the Output Control Package
 PCG for the Preconditioned Conjugate Gradient (PCG2 solver) Package
 GFD for the General Finite Difference Package
 HFB for the Horizontal Flow Barrier Package
 RES for the Reservoir Package
 STR for the Stream Routing Package
 IBS for the Interbed Storage Package
 CHD for the Constant Head Package
 FHB for the Specified Flow Package
 DATA for formatted (text) files such as those used to save formatted head and drawdown and for input of array data from files that are separate from the primary package input files.
 DATA(BINARY) for binary (unformatted) files such as those used to save cell-by-cell budget data and binary (unformatted) head and drawdown data.

Nunit is the Fortran unit to be used when reading from or writing to the file. Any legal unit number on the computer being used can be specified except units 94-99. Unit 99 is used for the name file and for reading arrays using the OPEN/CLOSE option. Units 97 and 98 are used for batch files as explained below. **Units 94-96 are used to create new input files when using the auto-conversion option (see Section 2.2.3).** Each file must have a unique unit number.

Fname is the filename of the file to be opened. No spaces or commas are allowed in the filename unless the filename is enclosed by single quotes (').

DIRECT is a keyword that can be used with DATA(BINARY) files to specify the file as a direct access binary file. *DIRECT* must be followed by Recl. (*Note: the Groundwater Vistas user interface (Environmental Simulations Inc, 2001), which is currently the Agency's preferred interface for MODFLOW modelling, only uses direct access files. The tick boxes specifying that model results are in double precision should all be ticked when importing model results. – This option does not work if the code has been compiled using the Compaq Fortran compiler*)

Recl is the record length of the direct access binary file. **For head, drawdown and cell-by-cell flow files the actual record length is calculated in the code, but a number should still be entered so that the file can be opened (recommended value: 1).**

Fname2 is used when an auto-conversion simulation is being run (see Section 2.2.3) to specify the names of the new Basic and Block Centred Flow files that are to be created by the code, and the names of the output files for the second simulation. Fname2 should be preceded by a 'greater than' character, '>', and a space. If the second set of binary output files is to be direct access, the keyword *DIRECT* and the record length Recl should be specified after Fname2.

Example NAME file:

```
LIST 10 Run38.out > Run38-part2.out
# Run 38 – VKD auto-conversion run using direct access binary
# files
BAS 20 Run38.bas > Run38-part2.bas
BCF 11 Run38.bcf > Run38-part2.bcf
DRN 13 ..\Run17\Run17.drn
RIV 14 ..\Run17\Run17.riv
WEL 12 ..\Run17\Run17.wel
RCH 18 ..\Run17\Run17.rch
OC 22 ..\Run17\Run17.oc
SIP 19 ..\Run17\Run17.sip
DATA(BINARY) 50 Run38.cbc DIRECT 1 > Run38-part2.cbc DIRECT 1
DATA(BINARY) 30 Run38.hds DIRECT 1 > Run38-part2.hds DIRECT 1
DATA(BINARY) 31 Run38.ddn DIRECT 1 > Run38-part2.ddn DIRECT 1
```

(note: the “..\Run17\” parts of the filenames above refer to input files in different directories)

6.3 Batch mode

Except as described below, MODFLOW will prompt the user to enter the name of the name file when MODFLOW is started. Once a name file is entered, MODFLOW will run without further user interaction.

Provision has been made to allow a series of simulations to be run without the need to manually restart MODFLOW for each simulation and respond to the prompt for the name file. This is called batch mode and is done through the use of a special file named `modflow.bf`. If this file exists in the user's current directory (where MODFLOW is run from) when MODFLOW is invoked, the user is not prompted for a name file. Instead, MODFLOW reads the names of the name files from `modflow.bf`. Each line of the file contains the name of a single name file, and each name can be up to 80 characters long.

When batch mode is used, a report file, named `modbatch.rpt`, is created. Before starting a simulation, the name of the name file is written to the report file. If the name file exists, the simulation is executed; when done, another message is written to the report file. If a name file does not exist, a message is written to the report file and processing continues with the next name file in `modflow.bf`.

When batch mode is used to run MODFLOW, two additional file units are used – 97 and 98. These units can not be used by any of the MODFLOW simulations. However, the file units used by one simulation can be the same as those used in any of the other simulations that are executed because each simulation is executed separately.

7 COMPILATION OPTIONS (SALFORD & COMPAQ)

The modified code has been compiled and tested using the Salford (Salford Software Ltd, 1996) and Compaq (Compaq Computer Corporation, 2000) FORTRAN compilers. The compiler control files are included on the CD which accompanies this report.

MODFLOW stores most of its variable arrays within a general array called the X-array. This array contains integer, real and double precision variables. This may cause problems with some FORTRAN compilers; for instance, the 16-bit Salford compiler (DBOS) requires an additional flag (NOCHECK) to be set in order for the code to work.

7.1 Salford

The following options have been used to compile the code using the Salford compiler (FTN77):

/INTL	Sets default integer length to four bytes.
/LIS	Produces a source listing file (to aid debugging).
/DEBUG	Causes the output of information to allow the use of source level debugging facilities.
/SAVE	Do not use the stack for storage of local variables and arrays. Otherwise dynamic storage is used for all local variables and arrays.
/ZEROISE	All static variables and arrays set to zero at start of execution.
/DREAL	changes all real variables (four byte) to double precision (eight byte)

All of the options above are optional, with the exception of INTL when compiling with the 16-bit compiler, and DREAL which is required to allow accurate calculation of variations in storage with depth.

7.2 Compaq

The only change made to the standard compiler options for the Compaq Visual Fortran compiler (Version 6.5) was to change the 'default real kind' from 4 to 8 (double precision).

Note: The option to write direct access binary output files does not work if the code has been compiled using the Compaq Fortran compiler.

To set up a workspace select:

- 'File' then 'New' then 'Projects' then 'FORTRAN Console Application'.
- Ensure 'Location' is path to directory containing source code.
- Ensure 'Project Name' is the same as directory name containing source code.
- Press return.
- Accept all other options to complete new workspace.
- Select 'Project' then 'Add to Project' then 'Files'.
- Select all source code files.
- The compiler options can be found in 'Project' then 'Settings' then 'FORTRAN'. Select the 'Fortran Data' category and change the 'default real kind' from 4 to 8 and click 'OK'.
- The executable can now be compiled under the 'build' menu (or by pressing F7).

8 PRACTICAL APPLICATION

8.1 Introduction

This section of the report is intended to provide guidance for modellers who are already fairly familiar with MODFLOW, who wish to use this modified version of the code to simulate aquifers where parameters vary with depth. The guidance presented here is based on the experience gained in the initial testing of the code and also on some modelling projects where the code is being further tested.

It should be noted that in some of the following subsections guidance has been aimed towards modellers using the Groundwater Vistas user interface (Environmental Simulations Inc, 2001), which is currently the Agency's preferred interface for MODFLOW modelling. It should be noted here that model results can only be imported into Groundwater Vistas if the binary output files are written as direct access files (see Section 6.2), and that the tick boxes specifying that the model output is in double precision should be checked on the Groundwater Vistas 'Import model results' dialogue box.

The following subsections include guidance on getting started, obtaining initial conditions for time variant simulations, converting existing steady-state MODFLOW models to VKD models, and converting steady-state models to time-variant models. This is followed by a summary of the effects of VKD and VSD on simulation results.

8.2 Getting started

The MODFLOW executable should either be located in the directory containing the model input files and run from there, or else can be located on the system path defined in the "autoexec.bat" file on the "C:\:" drive (or for windows NT/2000; under "Start" → "Settings" → "Control Panel" → "System" → [→ "Advanced"] "Environment"). To run the program bring up a command prompt or "DOS box", go to the directory containing the input files, and type in the name of the MODFLOW executable (eg, "MF-VKD1"). The user is then asked to enter name of the name file before the simulation commences.

The user should either use the executable included on the accompanying CD, or can compile the code themselves (see Section 7).

8.3 Obtaining initial conditions for a time variant VKD simulation

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

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

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

Environment Agency staff and consultants that have worked with the code have suggested different approaches to obtain a hydraulic conductivity profile and initial conditions for a time variant simulation where the water table and therefore transmissivity has a high seasonal variation.

One way to get an idea of how the hydraulic conductivity varies with depth is to obtain estimates of the transmissivity for high and low water table conditions, and then construct a hydraulic conductivity profile that gives the same high and low transmissivity values for the different water table levels. The transmissivity values can be estimated in the normal ways (ie, from observed groundwater gradients and flow estimates) and can be tested through model simulations. For example, the approach suggested to simulate the Upper Lee catchment involves bypassing the steady state phase of the modelling, and instead undertaking two time variant simulations with different distributions of specified transmissivities. The time variant simulations start with some representative initial heads (ie, contoured observed heads, or heads at surface elevation), and simulate a shortened historical sequence of recharge and abstraction. The first model has lower transmissivities, and is designed to reproduce the observed low flows over two or three years. The second model has higher transmissivities, designed to reproduce high flows. The transmissivity distributions are then compared, and combined to derive the VKD parameters. The advantages of this approach are likely to be:

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

The disadvantages are likely to be:

- The effects of the storage coefficients on simulation results may not be so easily differentiated from the effects of the VKD parameters. Some users report that this differentiation is relatively straightforward.
- It takes a relatively long time for the time-variant models to run and for any parameter changes to be assessed. This is not such a large problem with modern computers

Care needs to be taken to ensure that the model has reached dynamic balance.

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

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

The disadvantages of this approach are likely to be:

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

A third approach, which was employed for the Itchen and Mimram catchment models, consists in employing as initial conditions the heads produced in a time variant run where the model reaches dynamic balance based on a representative recharge pattern.

The above approaches avoid the use of the auto-conversion conversion option, and allow the VKD parameters to be input directly (rather than the base hydraulic conductivity being calculated by the MODFLOW code, resulting in 'measles plots' of hydraulic conductivity). From the points discussed above it is not immediately clear which of the three approaches is more useful. It was suggested that both the approaches should be investigated, and the relative merits of each could be compared once they had both been attempted.

8.4 Converting an existing steady-state MODFLOW-96 model to a VKD model: auto-conversion option

8.4.1 Setting up the MODFLOW input files

These notes describe how to convert an existing MODFLOW model to VKD model. The instructions below should be used in conjunction with the Input Instructions (Section 2.3).

All the following changes are made to the Block-Centred Flow (BCF) input file:

- Set the Steady State Flag (ISS) to 2 (if converting specified transmissivity layer(s) – LAYCON = 0 or 2) or 3 (if converting specified average hydraulic conductivity layer(s) – LAYCON = 1 or 3). This flag is the first number in the BCF file (row 1, columns 1 to 10).
- Set the Transmissivity Output Flag (ITRANS) to one. This allows the (inter-nodal) transmissivities calculated by VKD run to be compared against those from the specified transmissivity run (output to the listing file). This flag is located in columns 91 to 100 of row 1.
- Change the Layer Type (LAYCON) for the layer(s) of interest to 4 (unconfined VKD) or 5 (confined / unconfined VKD). Note: all other layer types (0 to 3) will be simulated in the normal way. These flags are located on the second line of the BCF file.
- Enter an array for the Bottom Elevations (BOT) if the original layer type was 0 or 2. If the original layer type was 1 or 3, the BCF file should already contain an array of bottom elevations. This array is located after the Transmissivity / Hydraulic Conductivity array.
- Enter an array for the Top Elevations (TOP) if specifying a confined / unconfined VKD type layer (LAYCON=5), and the original layer type was 0 or 1. If the original layer type was 2 or 3, the BCF file should already contain an array of top elevations. This array is located after the “Vcont” array if this is not the lowest layer in the model, or after the BOT array if it is the lowest layer – see the Input Instructions.
- Enter an array for the Thickness of the Upper Zone of the layer (the zone where hydraulic conductivity increases – commonly associated with the zone of fluctuation of groundwater heads). This array should be entered after all other arrays for the layer.
- Enter an array for the Hydraulic Conductivity Gradient Factor (VKGRAD – defined as the increase in hydraulic conductivity per unit rise in elevation, divided by the base hydraulic conductivity). This array should be placed after the upper thickness array.
- Enter an array for the Maximum Hydraulic Conductivity Factor (VKMAX – defined as the maximum hydraulic conductivity allowed in the upper zone of the layer, divided by the base hydraulic conductivity). This array should be placed after the VKGRAD array.
- It is a good idea to test out values for the parameters above, by checking the transmissivity given at different groundwater heads. This can be done by:
 - (i) calculating the transmissivity distribution for different heads in a spreadsheet and exporting it in matrix form as a text file
 - (ii) visualising the transmissivity distribution by importing the matrix contained in the text file in a spare property array in Groundwater Vistas (Environmental Simulations Inc, 2001)

Arrays of property values (upper thickness, hydraulic conductivity gradient factor, and maximum hydraulic conductivity factor) can be stored in spare property arrays in Groundwater Vistas (Environmental Simulations Inc, 2001) (eg, dispersivity, chemical reactions, and initial concentrations). The arrays can then be inserted into the BCF package by exporting them to a file [Props → Export → Property values (Matrix)...], and copying the array from that file to the relevant part of the BCF package. Note: if values are exported from Groundwater Vistas in exponential format, there will be 3 figures in the exponential part of the number. Although FORTRAN (the code MODFLOW is written in) usually reads and writes exponentials with two figures, it will also read three, so the values do not need to be changed.

Having made these changes, the BCF file should be ready for use. Save the file with a new filename. It is also good practice to create a new Basic (BAS) file with an updated title in the first two lines. The next step is to create a “name file” which contains a file descriptor (“LIST”, “BAS”, “WEL”, etc), a unit number (as shown in the [Model → Modflow → Packages] section in Groundwater Vistas), and a file name for each file used in the simulation (see Section 6.2). Binary output files (head, drawdown, and cell-by-cell flow files) should be identified by the descriptor “DATA(BINARY)”. Groundwater Vistas (Version 2) creates a name file (*.nam) when the MODFLOW input files are created, this file can be edited to use the filenames of the newly created files. All the other MODFLOW input files (WEL, RIV, DRN, etc) should be the same as for the original model.

Now run the MODFLOW-VKD application (using a DOS or command Box), and enter the name of the “name file” when prompted. Two simulations should run: the first a specified transmissivity or average hydraulic conductivity simulation, the second a VKD simulation.

8.4.2 Checking the simulation results

The outputs of the two simulations should be compared to verify that they give the same results (eg, inspect the drawdown file to check that the largest difference in head is small – say, less than 0.1 m). These results should also be compared against the original MODFLOW model (use the [Plot → File Operations → Compare Two Files...] option in Groundwater Vistas). Cell-by-cell flows can be compared in a similar way, and inter-nodal transmissivities can be compared in the output files from each simulation (if the Transmissivity Output Flag is not zero).

If there is a significant difference between the results of the two simulations, or if the second simulation does not converge, try changing the solver, or the solver options (PCG solver recommended). For example, the drawdowns produced in the second simulation will have values equal or very close to the opposite of the default value used for dry cells if dry cells are generated in the second simulation. In this case, decreasing the damping parameter reduces the oscillation of heads during the solving process and can avoid the generation of dry cells. Another way of avoiding differences between the results of the two simulations or non convergence is to reduce the Hydraulic Conductivity Gradient Factor and/or to increase the Upper Thickness, as this should reduce the non-linearity of the problem.

As well as checking the results of the two simulations, it is necessary to check the parameter values calculated by MODFLOW-VKD to make sure that the values themselves and their distribution are sensible. These parameters are the base hydraulic conductivities and the elevation of the change from constant to varying hydraulic conductivity (VMID – point of inflection). One way to do this is to copy the relevant arrays from the BCF package created by MODFLOW-VKD (second BCF file) into separate files, and import them into property arrays in Groundwater Vistas [Props → Import → Matrix...] (eg, the hydraulic conductivity and dispersivity property arrays). Then sort the arrays [Props → Property Values → Sort Zones], reset colours to grey scale [Props → Property Values → Reset Colors to Gray Scale], and reset the zone colours [Props → Property Values → Reset Zone Colors]. The property values can then be checked in either the database or by tracking the mouse pointer over the model cells.

8.5 Creating a time-variant VKD/VSD model from a steady-state VKD model

This Section describes how to set up the BCF file for a time variant VKD / VSD model. All the other packages (BAS, WEL, RIV, etc) should be created in the usual way (eg, using Groundwater Vistas (Environmental Simulations Inc, 2001), text editors, spreadsheets or FORTRAN routines). Make sure that the initial heads in the Basic (BAS) file are those calculated in the steady state VKD simulation (strictly speaking, these should be the heads produced from the second simulation, however, as the results of the two simulations should be the same, the heads produced from the first simulation can be used instead – reproduced in the 2nd Basic file).

Using the BCF package created in the steady state simulation (second BCF file) as a starting point, the following changes should be made:

- Change the steady state flag (ISS) to zero. This flag is the first number in the file (row 1, columns 1 to 10).
- Set the Transmissivity Output Flag (ITRANS) to zero. If this flag is non-zero, inter-nodal transmissivities are written to the output file every time step, leading to very large output files. This flag is located in columns 91 to 100 of row 1.
- Add the Primary Storage Coefficient array (Sf1). If the layer is unconfined (LAYCON = 1 or 4), this array contains values of Specific Yield. If the layer is confined or convertible (LAYCON = 0, 2, 3 or 5), this array contains values of Confined Storage Coefficient. This array should be placed before the (base) Hydraulic Conductivity array.
- If the layer type is convertible (LAYCON = 2, 3 or 5), add the Secondary Storage Coefficient (Sf2). This array is always Confined Storage Coefficient¹. This array should be placed before the Top Elevation array.
- Enter an array for the elevation of the point of inflection of unconfined storage (VSMID – defined as the elevation where storage changes from being constant to varying with depth). This array should be placed after the Maximum Hydraulic Conductivity Factor array.

¹ A possible exception to this might be in the case where a reduction in specific yield towards the top of the aquifer is being modelled (e.g. when simulating groundwater flooding). In this case the reduced Specific Yield should be entered in this array, and the “top” of the layer should be set to the elevation where the specific yield is believed to reduce. *Important note: using this approach means that the transmissivity will not increase once heads rise above the “top” of the layer. The modeller must verify that this approximation is valid (i.e. the contribution to the layer’s transmissivity above this point is negligible – however high the groundwater heads rise) before implementing it in the model.*

- Enter an array for the Storage Gradient Factor (VSGRAD – defined as the increase in specific yield per unit rise in elevation, divided by the base specific yield). This array should be placed after the VSMID array.
- Enter an array for the Maximum Storage Factor (VS MAX – defined as the maximum specific yield allowed in the upper zone of the layer, divided by the base specific yield). This array should be placed after the VSGRAD array.
- If no variation in storage is required, set VS MAX to one. It is good practice to examine the effects of VKD on simulation results before including variation in storage (VSD) as well.

Having made these changes, the BCF file should be ready for use. Save the file with a new filename. It is also good practice to create a new Basic (BAS) file with an updated title in the first two lines. The next step is to create a new “name file”. All the other MODFLOW input files (WEL, RIV, DRN, etc) should be the same as for a normal time-variant MODFLOW model.

Now run the MODFLOW-VKD application (using a DOS or command Box), and enter the name of the “name file” when prompted. A single VKD / VSD simulation should run. If the PCG solver is being used, the progress of the model is written to the screen (progress is not displayed for other solvers).

Due to the non-linearities of VSD, simulations with high values of VSGRAD are prone to instabilities, and may not converge easily. To avoid this, change the solver options. Alternatively, use low values of VSGRAD (between 0 and 0.5) and / or low values of VS MAX (between 1 and 1.5).

8.6 Effect of VKD/VSD on simulation results

Including variations in hydraulic properties with depth (VKD or VSD) in a numerical model effects the time-variant behaviour of the model, specifically the variability of the groundwater heads and flows. It should be recognised, however, that other model parameters can have similar effects on head and flow variability. One such parameter is the aquifer storage. Increasing the (non-depth dependant) storage in a model has the effect of reducing the variability of both heads and flows. Although these effects are different from those produced by a model with VKD (which increases flow variability and reduces head variation), it is not always easy to distinguish which parameters need changing without detailed analysis of the field data. Another important model input that has a direct effect of head and flow variability is the distribution of recharge through time. There are many different methods available for estimating recharge rates, but their time dependence is often harder to determine due especially to the effects of storage and throughflow in the unsaturated zone. In addition to the storage and recharge other parameters such as pumping rates, river coefficients and leakance between model layers can also affect head and flow variability, although some of these may only provide local changes.

8.6.1 Effect of VKD on simulation results

The effects of including a variation of hydraulic conductivity with depth are on the variation through time of groundwater heads and flows. Provided that the average transmissivity values remain the same, increasing the rate at which hydraulic conductivity reduces with depth has the effect of reducing head variations, whilst increasing the variation of flows to rivers and streams. However, although head variations are reduced in most areas, they are increased slightly near to outflow points such as rivers, streams and wells with variable pumping rates.

8.6.2 Effect of VSD on simulation results

Including variations in storage with depth also affect the variations of heads and flows through time. Provided that the storage at the average groundwater head level remains the same, increasing the rate at which storage reduces with depth has the effect of reducing heads slightly at both high and low points through time, whilst raising them slightly at intermediate points. The same is true for flows to rivers and streams.

9 POST PROCESSING UTILITIES

9.1 Introduction

As the modifications to the MODFLOW code have been tested using various different models, a number of post-processing utilities have been written and modified to aid the investigation of model results. This section includes descriptions of these utilities and instructions on how to use them.

9.2 Modifications to the USGS Zonebudget program (Zonebdgt8.exe)

Zonebudget is a FORTRAN program developed by the USGS to “compute and print volumetric budgets over subregions of a flow system that is being simulated using the USGS Modular Three-Dimensional Finite-Difference Ground-Water Flow Model” (Harbaugh, 1990).

At an early stage of the project it was necessary to know the water balance error at every node of the test models to insure that the acceptance criteria had been met. This was attempted using Zonebudget, with a different zone specified for each node in the model. However, the output files produced by the original version of the code were found to be very large and not very easy to interrogate, especially when investigating the results of time-variant models.

To avoid the problem of large files, and to make the program easier to use, the following changes were made:

- The format of the output file was changed to a table format that could be easily imported into a spreadsheet such as Excel.
- The option was added for the time step information to be read from the corresponding basic (BAS) file so that times can be included in the output files.
- The option was added for creating budget files for each zone and/or for each flow component.
- Modifications were made to allow either sequential or direct access cell-by-cell flow files to be read (although double precision cell-by-cell flow files are not recognised and must first be converted using the program ‘mf-convert.exe’).
- Additional changes were made to allow the program to read zone number outputs from Groundwater Vistas (Environmental Simulations Inc, 2001).

9.2.1 Inputs

Zonebudget should be run from a command prompt or DOS box by typing in the name of the executable file ('Zonebdgt8.exe'). Once the program starts the user is prompted to provide the following inputs:

1. ' Enter the name of a LISTING FILE for results:'

The user should enter the name of the main output file (eg, 'Run001.zbd'). The names of the individual files for each zone and flow component will be based on this filename (eg, 'Run001-Zone001.csv', 'Run001_____Storage.csv', etc).

2. ' Enter the name of the MODFLOW BAS file (reads timestep info; CR to skip):'

The user can either enter the name of the MODFLOW basic (BAS) file that was used in the simulation, or the input can be left blank (press the carriage return key). The bas file is used to calculate the simulation time corresponding to each timestep, if a bas file is not entered then zeros are entered in the time column of the output tables.

3. ' Enter the name of the file containing CELL-BY-CELL BUDGET TERMS:'

Here the name of the binary file containing cell-by-cell flows should be entered (eg, 'Run001.cbc'). This file can be either sequential access (as produced by MODFLOW-96) or direct access (as produced by MFWin32). MODFLOW-VKD can produce either sequential or direct access files.

If a bas file was not entered at step 2 then the following prompt is given:

- 3a. ' Enter number of rows, columns and layers:'

The user should then enter the number of rows, columns and layers in the model simulation (this information can be found in the bas file).

There is then a pause whilst the program scans the contents of the cell-by-cell flow file. This can sometimes take some time if it is a large file. A summary of the information in the cell-by-cell flow file is then printed to the screen.

4. ' Enter a TITLE to be printed in the listing:'

This title will be written in all the output files and can be used to provide information on the simulation and the zones used.

5. ' Enter the name of your ZONE INPUT FILE (CR for interactive):'

The zone input file can either be in the original format used for the USGS zonebudget program (Harbaugh, 1990), or a zone number file such as those produced by Groundwater Vistas (Environmental Simulations Inc, 2001). The zone number file contains the row, column and layer number of each cell followed by the zone number for that cell. The values for each cell should start on a new line of the file. All or some of the cells in the model domain can be specified (cells omitted from the zone number file will be considered as zone zero). The zone number file can be exported from Groundwater Vistas (Select the property zone to export then choose [P]rops]→[E]xport]→[Z]one Numbers...] from the menu. Don't tick the 'Export in Matrix Format' box).

If no zone input file name is entered then the user is prompted to enter zones interactively in blocks, specifying minimum and maximum rows, columns and layers for each block.

The highest zone number in the zone file is then written to the screen.

6. ' Remove obsolete columns from output files (Y/N)? '

If 'yes' is chosen for this option the output is initially written to temporary files. Once the program has finished running, these temporary files are scanned for columns that contain only zeros. These columns are removed from the final sets of output files. Any files in which all the columns contain zero values are permanently deleted.

7. 'Create output file for each zone?'

If 'yes' is typed for this option a different output file is produced for each specified zone.

8. 'Create output file for each boundary type?'

If 'yes' is typed for this option a different output file is produced for each component of the flow budget.

9. ' Choose the option for specifying when budgets are calculated:'

' A = ALL times stored in the budget file.'

' P = For each time stored in the budget file, PROMPT user.'

' L = Enter a LIST of times.'

The user should then specify which option is required. If the last option is chosen, up to ten different time steps can be specified.

The program now has enough information to process the cell-by-cell flow file. Messages are printed to the screen telling the user how far through the file the program is.

9.2.2 Outputs

The main output file (the listing file entered at the start of the program) contains a record of the inputs to the zonebudget program, which can be checked at a later date to verify all the inputs.

The remaining output files contain tables of flows for each zone and component of flow. Each file contains a header with the title that was entered at step 4, a description of which zone or component of flow the table is for, and a record of the name of the zone file. This is followed by a table of flows in and out of each zone and boundary condition against the stress period, time step and simulation time. The files are given the extension '.csv' so that they are automatically associated with Excel.

9.3 Program to calculate nodal water balance errors (WB-Error-dp.exe)

In order to facilitate the calculation of nodal water balance errors across a model, a FORTRAN program was written that reads the contents of a (direct access) binary cell-by-cell flow file, calculates both the absolute and percentage flow balance errors at every model node, and writes them to another cell-by-cell flow type binary file.

The program assumes that all the cell-by-cell flows (ie, from the BCF, stream and well packages, etc) have been written to the same file (on the same unit number). It also assumes that the file is in direct access format rather than sequential access format (see Section 6.2 and Section 9.4 below), and that it contains double precision values.

The program first asks the user to enter the name of the CBC (cell-by-cell flow) file to read. Once this has been entered (eg, 'Run001.cbb') the user is prompted for the name of the CBC type file of water balance errors that they want to create (eg, 'Run001-err.cbx'). This is followed by a request to choose from three different output options: absolute errors, percentage errors, or both. The program then reads the input CBC file, calculates the water balance errors for each node at each time step in the file, and writes the values to the output file. The output CBC file is in the same format as the input CBC file, but with title texts of 'Flow Balance Err' for absolute errors, and '% Flow Bal Err ' for percentage errors.

9.4 Programs to change the formats of MODFLOW binary output files

To avoid conflicts between versions of MODFLOW that use direct or sequential access binary files and utilities that use only one or the other, five FORTRAN programs have been written to convert MODFLOW binary output files from one format to the other. In addition to these two other utilities have been written to convert MODFLOW binary heads files to formats compatible with spreadsheets and plotting software. These seven programs are:

'cbc2dos.exe'	Converts CBC files from direct access to sequential access
'cbc2gv2.exe'	Converts CBC files from sequential access to direct access
'heads2dos.exe'	Converts heads (or drawdown) files from direct access to sequential access
'heads2gv2.exe'	Converts heads (or drawdown) files from sequential access to direct access
'mf-convert.exe'	Converts head, drawdown and cell-by-cell flow files between different combinations of direct and sequential access, and single and double precision.
'heads2csv.exe'	Converts heads files from direct/sequential format to comma separated variable (*.csv) format (text file for importing into spreadsheets)
'heads2tp.exe'	Converts heads files from direct/sequential format to TecPlot input format (*.plt)

All the programs require an input filename (of an existing MODFLOW output file) and an output filename. The first four programs also have the option to create a text (ASCII) file of head, drawdown or flow values. The last two programs require additional information on the specific time step or layer to export.

9.5 Programs to combine or split components of cell-by-cell flow files

The output options in MODFLOW allow the user to save the cell-by-cell flow terms from different packages to either one single file or many different files. Different post processing packages, such as those described above and others such as MODPATH, require all the cell-by-cell flows to be in a single file. Two FORTRAN programs have been written to either combine or split up cell-by-cell flow files depending on what is required. These programs are:

'cbc-split.exe'	Splits a single CBC flow file into different files containing one or more components of the flow.
'combine-cbb.exe'	Combines up to ten CBC flow files with the same model dimensions into one single CBC flow file.

Each program will prompt for the names of input and output filenames, and may require additional information or print an error message if a problem occurs. Both programs only work with single precision, direct access cell-by-cell flow files.

9.6 Program to extract time variant flows from the MODFLOW listing file (TVF-win5.exe)

This program reads the MODFLOW listing file and extracts the flow rates or cumulative volumes from the volumetric budget reported at the end of each time step. These values are then written to a new file in a table format, separated by commas, which can be opened in a spreadsheet, where the values can easily be plotted to show the variation of flows over time.

REFERENCES

Compaq Computer Corporation, 2000. *Compaq Visual Fortran Standard Version 6.5 User Guide*. Compaq Computer Corporation.

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

Environment Agency, 1999. *Representation of the Variation of Hydraulic Conductivity with Saturated Thickness in MODFLOW. Stages I & II. Code Changes and Testing Against Birmingham University Code*. Environment Agency. ISBN: 0 857 05194 7.

Environment Agency, 2002. *Enhancements to Modflow, variations in hydraulic conductivity and storage with depth*. Environment Agency. ISBN: 1 857 05765 1.

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

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

Harbaugh, A W, 1990, A computer program for calculating subregional water budgets using results from the U.S. Geological Survey modular three-dimensional ground-water flow model: U.S. Geological Survey Open-File Report 90-392, 46 p.

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

Hill M C, 1990. *Preconditioned Conjugate-Gradient 2 (PCG2), A Computer Program for Solving Ground-Water Flow Equations*. U.S. Geological Survey.

Kladias, M P & Ruskauff G J, 1996. *Computer Note on Implementing Spatially Variable Anisotropy in MODFLOW*. Geraghty and Miller, Inc and INTERA, Inc.

Lahey Computer Systems, Inc, 1995-1998. *FORTRAN 95 User Guide*. Lahey Computer Systems, Inc.

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

Owen M, and Robinson V K, 1978. *Characteristics and Yield in Fissured Chalk*. Institution of Civil Engineers, Symposium on Thames Groundwater Scheme, Paper 2, 33-49.

Prudic D E, 1989. *Documentation of a Computer Program to Simulate Stream-Aquifer Relations Using A Modular, Finite-Difference, Ground-Water Flow Model*. U.S. Geological Survey.

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

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

Rushton K R & Fawthrop N P, 1991. *Groundwater Support Of Stream Flows In Cambridge Area, UK*. Hydrological Basis of Ecologically Sound Management of Soil and Groundwater. IAHS Publication No. 202, 367-376.

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

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

Rushton K R, Smith E J & Tomlinson L M, 1982. *An Improved Understanding Of Flow in a Limestone Aquifer Using Field Evidence and Mathematical Models*. *Journal of the Institution of Water Engineers and Scientists*, Vol. 36, pp. 369 -387.

Salford Software Ltd, 1996. *FTN77 User's Guide*. Salford Software Ltd.

Salmon S, Chadha D & Smith D, 1996. *Development of a Groundwater Resource Model for the Yorkshire Chalk*. *Journal of the Chartered Institution of Water and Environmental Management*, 10, pp. 37-48.

Southern Water Authority, 1979. *Itchen Groundwater Regulation Scheme; Final report on the Candover Pilot Scheme*. Southern Water Authority, Hampshire.

APPENDIX A
Modified computer code for BCF package
with changes highlighted

COMPILER OPTIONS: listing intl no_persist nodclvar nomap nocheck logl dynm offset dreal noansi
nopagethrow

nosilent no_optimise warn73 nolink no_link

```
0001 C-Changes to the code are highlighted with the following headings:
0002 C
0003 C-Environment Agency (UK)-0.General change to enable new options>>>>>>>>
0004 C-Environment Agency (UK)-1.Variable hydraulic cond. w/depth (VKD)>>>>>
0005 C-Environment Agency (UK)-2.Variable storage with depth (VSD)>>>>>>>>>>
0006 C-Environment Agency (UK)-3.Auto-conversion for steady state VKD>>>>>>>>
0007 C-Environment Agency (UK)-4.Spatially variable anisotropy>>>>>>>>>>>>
0008 C-Environment Agency (UK)-5.Inter-nodal transmissivities>>>>>>>>>>>>
0009 C-Environment Agency (UK)-6.X & Y-dir transmissivities>>>>>>>>>>>>>>
0010 C-Environment Agency (UK)-7.Explicit transmissivity calculation>>>>>>>>>
0011 C-Environment Agency (UK)-8.Output calculated transmissivities>>>>>>>>>>
0012 C-Environment Agency (UK)-9.Bug fix>>>>>>>>>>>>>>>>>>>>>>>>>>>>
0013 C-Environment Agency (UK)-10.K gradient independant of kbase>>>>>>>>>>>>
0014 C-Environment Agency (UK)-11.Output calc trans to binary file>>>>>>>>>>>
0015 C-Environment Agency (UK)-12.Bug fix>>>>>>>>>>>>>>>>>>>>>>>>>>>
0016 C
0017 C These headings are followed by the original USGS MODFLOW-96 code
0018 C (commented out), followed by the modified code. All the code changes
0019 C are followed by the following:
0020 C
0021 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<<
0022 C
0023 C-Environment Agency (UK)-0.General change to enable new options>>>>>>>>
0024 c SUBROUTINE BCF5AL (ISUM, LENX, LCSC1, LCHY, LCBOT, LCTOP, LCSC2, LCTRPY,
0025 c 1 IN, ISS, NCOL, NROW, NLAY, IOUT, IBCFCB, LCWETD, IWDFLG, LCCVWD,
0026 c 2 WETFCT, IWETIT, IHDWET, HDRY, IAPART, IFREFM)
0027 C-Environment Agency (UK)-10.K gradient independant of kbase>>>>>>>>>>>>
0028 c SUBROUTINE BCF5AL (ISUM, LENX, LCSC1, LCHY, LCBOT, LCTOP, LCSC2, LCTRPY,
0029 c 1 IN, ISS, NCOL, NROW, NLAY, IOUT, IBCFCB, LCWETD, IWDFLG, LCCVWD,
0030 c 2 WETFCT, IWETIT, IHDWET, HDRY, IAPART, IFREFM, itrpy, lckgrad, ihold,
0031 c 3 itrans, lcmid, lckmax, lcsgrad, lcsmax, lcsmid)
0032 SUBROUTINE BCF5AL (ISUM, LENX, LCSC1, LCHY, LCBOT, LCTOP, LCSC2, LCTRPY,
0033 c 1 IN, ISS, NCOL, NROW, NLAY, IOUT, IBCFCB, LCWETD, IWDFLG, LCCVWD,
0034 c 2 WETFCT, IWETIT, IHDWET, HDRY, IAPART, IFREFM, itrpy, lckgrad, ihold,
0035 c 3 itrans, lcmid, lckmax, lcsgrad, lcsmax, lcsmid, ikbase)
0036 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<<
0037 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<<
0038 C
0039 C-----VERSION 1431 20FEB1996 BCF5AL
0040 C *****
0041 C ALLOCATE ARRAY STORAGE FOR BLOCK-CENTERED FLOW PACKAGE
0042 C *****
0043 C
0044 C SPECIFICATIONS:
0045 C -----
0046 COMMON /FLWCOM/LAYCON(200)
0047 COMMON /FLWAVG/LAYAVG(200)
0048 C-Environment Agency (UK)-5.Inter-nodal transmissivities>>>>>>>>>>>>>>
0049 c CHARACTER*12 AVGNAM(4)
0050 c DATA AVGNAM/'HARMONIC ','ARITHMETIC ',
0051 c 1 'LOGARITHMIC ','*UNCONFINED*'/
0052 CHARACTER*12 AVGNAM(5)
0053 DATA AVGNAM/'HARMONIC ','ARITHMETIC ', AT 001B
0054 c 1 'LOGARITHMIC ','*UNCONFINED*',
0055 c 2 'INTERNODAL '/
0056 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<<
0057 C -----
0058 C
0059 C1-----IDENTIFY PACKAGE
0060 WRITE(IOUT,1) IN AT 001B
0061 C-Environment Agency (UK)-0.General change to enable new options>>>>>>>>
0062 c 1 FORMAT(1X,/1X,'BCF5 -- BLOCK-CENTERED FLOW PACKAGE, VERSION 5',
0063 c 1', 9/1/93',' INPUT READ FROM UNIT',I3)
0064 C-Environment Agency (UK)-10.K gradient independant of kbase>>>>>>>>>>>>
0065 c 1 FORMAT(1X,/1X,'BCF-VKD1 -- BLOCK-CENTERED FLOW PACKAGE WITH ',
0066 c 1'VARIABLE HYDRAULIC CONDUCTIVITY WITH DEPTH (VKD), VERSION 1',
0067 c 1', 18/7/01',' INPUT READ FROM UNIT',I3)
0068 c 1 FORMAT(1X,/1X,'BCF-VKD3 -- BLOCK-CENTERED FLOW PACKAGE WITH ', AT 0051
0069 c 1'VARIABLE HYDRAULIC CONDUCTIVITY WITH DEPTH (VKD), VERSION 5',
0070 c 1', 16/5/03',' INPUT READ FROM UNIT',I3)
0071 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<<
0072 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<<
0073 C
0074 C2-----READ AND PRINT ISS (STEADY-STATE FLAG), IBCFCB (FLAG FOR
0075 C2-----PRINTING OR UNIT# FOR RECORDING CELL-BY-CELL FLOW TERMS), HDRY
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0076 C2----- (HEAD AT CELLS THAT CONVERT TO DRY), WETTING PARAMETERS,
0077 c2----- anisotropy option, explicit transmissivity calculation option,
0078 c2----- and transmissivity output option.
0079 c
0080 C-Environment Agency (UK)-0.General change to enable new options>>>>>>>>>>
0081 c IF (IFREFM.EQ.0) THEN
0082 c READ (IN, '(2I10,F10.0,I10,F10.0,2I10)')
0083 c 1 ISS, IBCFCB, HDRY, IWDFLG, WETFCT, IWETIT, IHDWET
0084 c ELSE
0085 c READ (IN, *) ISS, IBCFCB, HDRY, IWDFLG, WETFCT, IWETIT, IHDWET
0086 c END IF
0087 C-Environment Agency (UK)-10.K gradient independant of kbase>>>>>>>>>>>>>>
0088 c IF (IFREFM.EQ.0) THEN
0089 c READ (IN, '(2I10,F10.0,I10,F10.0,5I10)')
0090 c 1 ISS, IBCFCB, HDRY, IWDFLG, WETFCT, IWETIT, IHDWET, itrpy
0091 c 2 , ihold, itrans
0092 c ELSE
0093 c READ (IN, *) ISS, IBCFCB, HDRY, IWDFLG, WETFCT, IWETIT, IHDWET, itrpy
0094 c 1 , ihold, itrans
0095 c END IF
0096 IF (IFREFM.EQ.0) THEN AT 010C
0097.01 READ (IN, '(2I10,F10.0,I10,F10.0,6I10)') AT 0118
0098.01 1 ISS, IBCFCB, HDRY, IWDFLG, WETFCT, IWETIT, IHDWET, itrpy
0099.01 2 , ihold, itrans, ikbase
0100.01 ELSE AT 021F
0101.01 READ (IN, *) ISS, IBCFCB, HDRY, IWDFLG, WETFCT, IWETIT, IHDWET, itrpy AT 0224
0102.01 1 , ihold, itrans, ikbase
0103.01 END IF AT 02EE
0104.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0105.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0106 IF (ISS.EQ.0) WRITE (IOUT,3) AT 02EE
0107 3 FORMAT (1X, 'TRANSIENT SIMULATION') AT 0320
0108 IF (ISS.NE.0) WRITE (IOUT,4) AT 034B
0109 4 FORMAT (1X, 'STEADY-STATE SIMULATION') AT 037D
0110 IF (IBCFCB.LT.0) WRITE (IOUT,8) AT 03AC
0111 8 FORMAT (1X, 'CONSTANT-HEAD CELL-BY-CELL FLOWS WILL BE PRINTED',
0112 1 ' WHEN IBCFCFL IS NOT 0')
0113 IF (IBCFCB.GT.0) WRITE (IOUT,9) IBCFCB AT 043F
0114 9 FORMAT (1X, 'CELL-BY-CELL FLOWS WILL BE SAVED ON UNIT', I3) AT 0481
0115 WRITE (IOUT,11) HDRY AT 04C6
0116 11 FORMAT (1X, 'HEAD AT CELLS THAT CONVERT TO DRY=', G13.5) AT 04FC
0117 IF (IWDFLG.NE.0) GO TO 35 AT 053D
0118 WRITE (IOUT,12) AT 0549
0119 12 FORMAT (1X, 'WETTING CAPABILITY IS NOT ACTIVE') AT 056F
0120 GO TO 39 AT 05A6
0121 C
0122 35 WRITE (IOUT,36) AT 05AB
0123 36 FORMAT (1X, 'WETTING CAPABILITY IS ACTIVE') AT 05D1
0124 IF (IWETIT.LE.0) IWETIT=1 AT 0604
0125 WRITE (IOUT,37) WETFCT, IWETIT AT 0616
0126 37 FORMAT (1X, 'WETTING FACTOR=', F10.5, AT 065C
0127 1 ' WETTING ITERATION INTERVAL=', I4)
0128 WRITE (IOUT,38) IHDWET AT 06B5
0129 38 FORMAT (1X, 'FLAG THAT SPECIFIES THE EQUATION TO USE FOR HEAD',
0130 1 ' AT WETTED CELLS=', I4) AT 06EB
0131 C
0132 C3----- STOP THE SIMULATION IF THERE ARE MORE THAN 200 LAYERS.
0133 39 IF (NLAY.LE.200) GO TO 50 AT 074E
0134 WRITE (IOUT,41) AT 075D
0135 41 FORMAT (1X, /1X, 'YOU HAVE SPECIFIED MORE THAN 200 MODEL LAYERS'/1X,
0136 1 'SPACE IS RESERVED FOR A MAXIMUM OF 200 LAYERS IN ARRAYS LAYCON',
0137 2 ' AND LAYAVG')
0138 STOP AT 082A
0139 C
0140 C4----- READ LAYCON & PRINT TITLE FOR LAYCON TABLE.
0141 C-Environment Agency (UK)-10.K gradient independant of kbase>>>>>>>>>>>>>>
0142 c 50 IF (IFREFM.EQ.0) THEN
0143 50 if (ikbase.ne.0.and.(iss.eq.2.or.iss.eq.3)) then AT 083D
0144.01 write (iout,51) AT 085E
0145.01 51 format (1X, /1X, 'YOU HAVE SPECIFIED VKGRAD TO BE INDEPENDANT OF'/1X,
0146.01 1 'K BASE, BUT USING THE AUTOMATIC CONVERSION OPTION. THIS'/1X,
0147.01 2 'COMBINATION IS NOT SUPPORTED. VKGRAD WILL BE A MULTIPLE OF'/1X,
0148.01 3 'K BASE')
0149.01 ikbase=0 AT 096D
0150.01 endif AT 0976
0151 IF (IFREFM.EQ.0) THEN AT 0976
0152 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0153.01 READ (IN, '(40I2)') (LAYCON(I), I=1, NLAY) AT 0982
0154.01 ELSE AT 0A01
0155.01 READ (IN, *) (LAYCON(I), I=1, NLAY) AT 0A06
0156.01 END IF AT 0A64
0157 WRITE (IOUT,52) AT 0A64

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0319 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0320 DOUBLE PRECISION HNEW
0321 C
0322 C-Environment Agency (UK)-0.General change to enable new options>>>>>>>
0323 c DIMENSION HNEW(NCOL,NROW,NLAY),SC1(NCOL,NROW,NLAY),
0324 c 1 HY(NCOL,NROW,NLAY),CR(NCOL,NROW,NLAY),CC(NCOL,NROW,NLAY),
0325 c 2 CV(NCOL,NROW,NLAY),DELR(NCOL),DELC(NROW),BOT(NCOL,NROW,NLAY),
0326 c 3 TOP(NCOL,NROW,NLAY),SC2(NCOL,NROW,NLAY),TRPY(NLAY),
0327 c 4 IBOUND(NCOL,NROW,NLAY),WETDRY(NCOL,NROW,NLAY),
0328 c 5 CVWD(NCOL,NROW,NLAY)
0329 DIMENSION HNEW(NCOL,NROW,NLAY),SC1(NCOL,NROW,NLAY),
0330 1 HY(NCOL,NROW,NLAY),CR(NCOL,NROW,NLAY),CC(NCOL,NROW,NLAY),
0331 2 CV(NCOL,NROW,NLAY),DELR(NCOL),DELC(NROW),BOT(NCOL,NROW,NLAY),
0332 3 TOP(NCOL,NROW,NLAY),SC2(NCOL,NROW,NLAY),TRPY(ncol,nrow,nlay),
0333 4 IBOUND(NCOL,NROW,NLAY),WETDRY(NCOL,NROW,NLAY),
0334 5 CVWD(NCOL,NROW,NLAY),vkgrad(ncol,nrow,nlay),
0335 6 vmid(ncol,nrow,nlay),vkmax(ncol,nrow,nlay),
0336 7 vsgrad(ncol,nrow,nlay),vsmid(ncol,nrow,nlay),
0337 8 vsmid(ncol,nrow,nlay)
0338 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0339 C
0340 COMMON /FLWCOM/LAYCON(200)
0341 C
0342 DATA ANAME(1) /' PRIMARY STORAGE COEF'/ AT 0085
0343 DATA ANAME(2) /' TRANSMIS. ALONG ROWS'/ AT 0085
0344 DATA ANAME(3) /' HYD. COND. ALONG ROWS'/ AT 0085
0345 DATA ANAME(4) /'VERT HYD COND /THICKNESS'/ AT 0085
0346 DATA ANAME(5) /' BOTTOM'/ AT 0085
0347 DATA ANAME(6) /' TOP'/ AT 0085
0348 DATA ANAME(7) /' SECONDARY STORAGE COEF'/ AT 0085
0349 DATA ANAME(8) /' COLUMN TO ROW ANISOTROPY'/ AT 0085
0350 DATA ANAME(9) /' DELR'/ AT 0085
0351 DATA ANAME(10) /' DELC'/ AT 0085
0352 DATA ANAME(11) /' WETDRY PARAMETER'/ AT 0085
0353 C-Environment Agency (UK)-0.General change to enable new options>>>>>>>
0354 data aname(12) /'HYD COND GRADIENT FACTOR'/ AT 0085
0355 data aname(13) /' THICKNESS OF UPPER ZONE'/ AT 0085
0356 DATA ANAME(14) /' BOTTOM'/ AT 0085
0357 data aname(15) /' TRANSMIS. ALONG COLUMNS'/ AT 0085
0358 data aname(16) /'HYD. COND. ALONG COLUMNS'/ AT 0085
0359 data aname(17) /'ELEVATION OF CHANGE IN K'/ AT 0085
0360 data aname(18) /' MAXIMUM HYD COND FACTOR'/ AT 0085
0361 data aname(19) /' STORAGE GRADIENT FACTOR'/ AT 0085
0362 data aname(20) /' MAXIMUM STORAGE FACTOR'/ AT 0085
0363 data aname(21) /'ELEVATION OF CHANGE IN S'/ AT 0085
0364 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0365 C -----
0366 C
0367 C1-----READ TRPY,DELR,DELC.
0368 C-Environment Agency (UK)-4.Spatially variable anisotropy>>>>>>>>>>>>>
0369 c CALL UIDREL(TRPY,ANAME(8),NLAY,IN,IOUT)
0370 if(itrpy.eq.0)then AT 0085
0371.01 loc=1 AT 0091
0372.01 call u2drel(trpy(1,1,1),aname(8),loc,nlay,loc,in,iout) AT 009B
0373.01 elseif(itrpy.ne.2)then AT 00E9
0374.01 do 23 k=1,nlay AT 00FA
0375.02 call u2drel(trpy(1,1,k),aname(8),nrow,ncol,k,in,iout) AT 0127
0376.02 23 continue AT 0175
0377.01 endif AT 0177
0378.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0379 CALL UIDREL(DELR,ANAME(9),NCOL,IN,IOUT) AT 0177
0380 CALL UIDREL(DELC,ANAME(10),NROW,IN,IOUT) AT 0198
0381 C
0382 C2-----READ ALL PARAMETERS FOR EACH LAYER.
0383 KT=0 AT 01B9
0384 KB=0 AT 01C3
0385 C-Environment Agency (UK)-1.Variable hydraulic cond. w/depth (VKD)>>>>>
0386 kg=0 AT 01CD
0387 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0388 DO 200 K=1,NLAY AT 01D7
0389.01 KK=K AT 0204
0390.01 C
0391.01 C2A-----FIND ADDRESS OF EACH LAYER IN THREE DIMENSION ARRAYS.
0392.01 C-Environment Agency (UK)-1.Variable hydraulic cond. w/depth (VKD)>>>>>
0393.01 C IF(LAYCON(K).EQ.1 .OR. LAYCON(K).EQ.3) KB=KB+1
0394.01 C IF(LAYCON(K).EQ.2 .OR. LAYCON(K).EQ.3) KT=KT+1
0395.01 IF(LAYCON(K).EQ.1 .OR. LAYCON(K).EQ.3 .or. laycon(k).eq.4 .or. AT 020A
0396.01 1 laycon(k).eq.5) KB=KB+1
0397.01 IF(LAYCON(K).EQ.2 .OR. LAYCON(K).EQ.3 .or. laycon(k).eq.5) KT=KT+1 AT 0248
0398.01 if(laycon(k).eq.4 .or. laycon(k).eq.5) kg=kg+1 AT 027E
0399.01 C
0400.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<

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0561          SUBROUTINE BCF5AD ( IBOUND,HOLD,BOT,WETDRY,IWDFLG,ISS,
0562          1          NCOL,NROW,NLAY)
0563          C
0564          C-----VERSION 1659 30OCT1992 BCF5AD
0565          C *****
0566          C      SET HOLD TO BOT WHENEVER A WETTABLE CELL IS DRY
0567          C *****
0568          C
0569          C          SPECIFICATIONS:
0570          C -----
0571          C
0572          DIMENSION IBOUND (NCOL,NROW,NLAY) ,HOLD (NCOL,NROW,NLAY) ,
0573          1          BOT (NCOL,NROW,NLAY) ,WETDRY (NCOL,NROW,NLAY)
0574          C
0575          COMMON /FLWCOM/LAYCON (200)
0576          C -----
0577          C
0578          C1-----RETURN IF STEADY STATE OR IF NOT USING WETTING CAPABILITY
0579          IF (IWDFLG.EQ.0 .OR. ISS.NE.0) RETURN                                AT 004C
0580          C
0581          C2-----LOOP THROUGH ALL LAYERS TO SET HOLD=BOT IF A WETTABLE CELL IS DRY
0582          ZERO=0.                                                            AT 0064
0583          KB=0                                                                AT 0072
0584          DO 100 K=1,NLAY                                                    AT 0079
0585          C
0586          C2A-----SKIP LAYERS THAT CANNOT CONVERT BETWEEN WET AND DRY
0587          C-Environment Agency (UK)-1.Variable hydraulic cond. w/depth (VKD)>>>>>
0588          c      IF (LAYCON (K) .NE.3 .AND. LAYCON (K) .NE.1) GO TO 100
0589.01          IF (LAYCON (K) .NE.3 .AND. LAYCON (K) .NE.1 .and. laycon (k) .ne.4 .and.    AT 0092
0590.01          1          laycon (k) .ne.5) GO TO 100
0591.01          C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0592.01          KB=KB+1                                                        AT 00CA
0593.01          DO 90 I=1,NROW                                                AT 00CD
0594.02          DO 90 J=1,NCOL                                                AT 00EB
0595.02          C
0596.02          C2B-----SKIP CELLS THAT ARE CURRENTLY WET OR ARE NOT WETTABLE
0597.03          IF ( IBOUND (J,I,K) .NE.0) GO TO 90                          AT 0109
0598.03          IF (WETDRY (J,I,KB) .EQ.ZERO) GO TO 90                       AT 012D
0599.03          C
0600.03          C2C-----SET HOLD=BOT
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
0601.03          HOLD (J,I,K)=BOT (J,I,KB)                                     AT 0157
0602.03          90 CONTINUE                                                  AT 0195
0603.01          100 CONTINUE                                                AT 019F
0604.01          C
0605.01          C3-----RETURN
0606          RETURN                                                            AT 01A4
0607          END                                                            AT 01A9
0608          C-Environment Agency (UK)-0.General change to enable new options>>>>>>>
0609          c      SUBROUTINE BCF5FM (HCOF,RHS,HOLD,SC1,HNEW,IBOUND,CR,CC,CV,HY,TRPY,
0610          c      1          BOT, TOP, SC2, DELR, DELC, DELT, ISS, KITER, KSTP, KPER,
0611          c      2          NCOL,NROW,NLAY, IOUT,WETDRY,IWDFLG,CVWD,
0612          c      3          WETFCT,IWETIT,IHDWET,HDRY,BUFF,itrpy,vkgrad,ihold,
0613          SUBROUTINE BCF5FM (HCOF,RHS,HOLD,SC1,HNEW,IBOUND,CR,CC,CV,HY,TRPY,
0614          1          BOT, TOP, SC2, DELR, DELC, DELT, ISS, KITER, KSTP, KPER,
0615          2          NCOL,NROW,NLAY, IOUT,WETDRY,IWDFLG,CVWD,
0616          3          WETFCT,IWETIT,IHDWET,HDRY,BUFF,itrpy,vkgrad,ihold,
0617          4          vmid,vkmax,vsgrad,vsmid)
0618          C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0619          C-----VERSION 1500 29JUNE1993 BCF5FM
0620          C *****
0621          C      ADD LEAKAGE CORRECTION AND STORAGE TO HCOF AND RHS, AND CALCULATE
0622          C      CONDUCTANCE AS REQUIRED
0623          C *****
0624          C
0625          C          SPECIFICATIONS:
0626          C -----
0627          C-Environment Agency (UK)-2.Variable storage with depth (VSD)>>>>>>>>>
0628          c      DOUBLE PRECISION HNEW
0629          DOUBLE PRECISION HNEW,htmp,vm,vsm,vsg,esm,bt,stamp,sold,snew,scof,
0630          1          rho1,rho2,tp
0631          C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0632          C
0633          C-Environment Agency (UK)-0.General change to enable new options>>>>>>>
0634          c      DIMENSION HCOF (NCOL,NROW,NLAY) ,RHS (NCOL,NROW,NLAY) ,
0635          c      1          HOLD (NCOL,NROW,NLAY) ,SC1 (NCOL,NROW,NLAY) ,HNEW (NCOL,NROW,NLAY) ,
0636          c      2          IBOUND (NCOL,NROW,NLAY) ,CR (NCOL,NROW,NLAY) ,
0637          c      3          CC (NCOL,NROW,NLAY) ,CV (NCOL,NROW,NLAY) ,HY (NCOL,NROW,NLAY) ,

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0638      c      4      TRPY (NLAY) , BOT (NCOL, NROW, NLAY) , TOP (NCOL, NROW, NLAY) , DELR (NCOL) ,
0639      c      5      DELC (NROW) , SC2 (NCOL, NROW, NLAY) , WETDRY (NCOL, NROW, NLAY) ,
0640      c      6      CVWD (NCOL, NROW, NLAY) , BUFF (NCOL, NROW, NLAY)
0641      DIMENSION HCOF (NCOL, NROW, NLAY) , RHS (NCOL, NROW, NLAY) ,
0642      1      HOLD (NCOL, NROW, NLAY) , SC1 (NCOL, NROW, NLAY) , HNEW (NCOL, NROW, NLAY) ,
0643      2      IBOUND (NCOL, NROW, NLAY) , CR (NCOL, NROW, NLAY) ,
0644      3      CC (NCOL, NROW, NLAY) , CV (NCOL, NROW, NLAY) , HY (NCOL, NROW, NLAY) ,
0645      4      TRPY (ncol, nrow, nlay) , BOT (NCOL, NROW, NLAY) , TOP (NCOL, NROW, NLAY) ,
0646      5      DELR (NCOL) , DELC (NROW) , SC2 (NCOL, NROW, NLAY) ,
0647      6      WETDRY (NCOL, NROW, NLAY) , CVWD (NCOL, NROW, NLAY) ,
0648      7      BUFF (NCOL, NROW, NLAY) , vkgrad (ncol, nrow, nlay) ,
0649      8      vmid (ncol, nrow, nlay) , vkmax (ncol, nrow, nlay)
0650      dimension vsgrad (ncol, nrow, nlay) , vsmax (ncol, nrow, nlay) ,
0651      1      vsmid (ncol, nrow, nlay)
0652      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0653      C
0654      COMMON /FLWCOM/LAYCON(200)
0655      C -----
0656      KB=0
0657      KT=0
0658      C-Environment Agency (UK)-1.Variable hydraulic cond. w/depth (VKD)>>>>>
0659      kg=0
0660      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0661      ONE=1.
0662      TLED=ONE/DELT
0663      C
0664      C1-----FOR EACH LAYER: IF T VARIES CALCULATE HORIZONTAL CONDUCTANCES
0665      DO 100 K=1,NLAY
0666.01      KK=K
0667.01      C-Environment Agency (UK)-1.Variable hydraulic cond. w/depth (VKD)>>>>>
0668.01      c      IF (LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.2) KT=KT+1
0669.01      IF (LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.2 .or. laycon(k).eq.5) KT=KT+1
0670.01      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0671.01      C
0672.01      C1A----IF LAYER TYPE IS NOT 1, 3, 4 or 5 THEN SKIP THIS LAYER.
0673.01      C-Environment Agency (UK)-1.Variable hydraulic cond. w/depth (VKD)>>>>>
0674.01      c      IF (LAYCON(K).NE.3 .AND. LAYCON(K).NE.1) GO TO 100
0675.01      IF (LAYCON(K).NE.3 .AND. LAYCON(K).NE.1 .and. laycon(k).ne.4 .and.
0676.01      1      laycon(k).ne.5) GO TO 100
0677.01      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0678.01      KB=KB+1
0679.01      C-Environment Agency (UK)-1.Variable hydraulic cond. w/depth (VKD)>>>>>
0680.01      if (laycon(k).eq.4 .or. laycon(k).eq.5) kg=kg+1
0681.01      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0682.01      C
0683.01      C1B----FOR LAYER TYPES 1, 3, 4 & 5 CALL SBCF5H TO CALCULATE
0684.01      C1B----HORIZONTAL CONDUCTANCES.
0685.01      C-Environment Agency (UK)-0.General change to enable new options>>>>>>>
0686.01      c      CALL SBCF5H (HNEW, IBOUND, CR, CC, CV, HY, TRPY, DELR, DELC, BOT, TOP,
0687.01      c      1      KK, KB, KT, KITER, KSTP, KPER, NCOL, NROW, NLAY, IOUT, WETDRY, IWDFLG,
0688.01      c      2      CVWD, WETFACT, IWETIT, IHDWET, HDRY, BUFF)
0689.01      CALL SBCF5H (HNEW, IBOUND, CR, CC, CV, HY, TRPY, DELR, DELC, BOT, TOP,
0690.01      1      KK, KB, KT, KITER, KSTP, KPER, NCOL, NROW, NLAY, IOUT, WETDRY, IWDFLG,
0691.01      2      CVWD, WETFACT, IWETIT, IHDWET, HDRY, BUFF, itrpy, vkgrad, kg, hold, ihold,
0692.01      3      iss, vmid, vkmax)
0693.01      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0694.01      100 CONTINUE
0695.01      C
0696.01      C2-----IF THE SIMULATION IS TRANSIENT ADD STORAGE TO HCOF AND RHS
0697      IF (ISS.NE.0) GO TO 201
0698      KT=0
0699      C-Environment Agency (UK)-2.Variable storage with depth (VSD)>>>>>>>>>
0700      kb=0
0701      kg=0
0702      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0703      DO 200 K=1,NLAY
0704      C
0705      C3-----SEE IF THIS LAYER IS CONVERTIBLE OR NON-CONVERTIBLE.
0706.01      IF (LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.2) GO TO 150
0707.01      c
0708.01      C-Environment Agency (UK)-2.Variable storage with depth (VSD)>>>>>>>>>
0709.01      c3a----See if This Layer has Varying Storage with Depth (VSD)
0710.01      if (laycon(k).eq.4.or.laycon(k).eq.5) goto 400
0711.01      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0712.01      C4-----NON-CONVERTIBLE LAYER, SO USE PRIMARY STORAGE
0713.01      DO 140 I=1,NROW
0714.02      DO 140 J=1,NCOL
0715.03      IF (IBOUND(J, I, K).LE.0) GO TO 140
0716.03      RHO=SC1(J, I, K)*TLED
0717.03      HCOF(J, I, K)=HCOF(J, I, K)-RHO
0718.03      RHS(J, I, K)=RHS(J, I, K)-RHO*HOLD(J, I, K)
0719.03      140 CONTINUE

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AT 0085
AT 008F
AT 0099
AT 00A3
AT 00B7
AT 00C9
AT 00F1
AT 00F7
AT 0127
AT 0165
AT 016B
AT 023B
AT 0240
AT 024C
AT 0256
AT 0260
AT 026A
AT 0297
AT 02B3
AT 02CF
AT 02FC
AT 0329
AT 0362
AT 039B
AT 03CE
AT 0411

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0962.03         if (itrpy.ne.2) then                                AT 0326
0963.04             t1=t1*trpy(j,i,k)                            AT 0332
0964.04             t2=t2*trpy(j,i+1,k)                          AT 0359
0965.04         endif                                            AT 0380
0966.03             CC(J,I,K)=2*T2*T1*DELR(J)/(T1*DELC(I+1)+T2*DELC(I)) AT 0380
0967.03         endif                                            AT 03D8
0968.03 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0969.02     40 CONTINUE                                          AT 03D8
0970.02     C
0971.02 C5-----RETURN
0972         RETURN                                            AT 03E2
0973         END                                              AT 03E7

0974         SUBROUTINE SBCF5B(HNEW,IBOUND,CR,CC,CV,TOP,NCOL,NROW,NLAY,KSTP,
0975     1         KPER,IBCFCB,BUFF,IOUT,ICBCFL,DELT,PERTIM,TOTIM,
0976     2         IDIR,IBDRET,ICHFLG,IC1,IC2,IR1,IR2,IL1,IL2)
0977     C
0978     C-----VERSION 1308 28JUNE1993 SBCF5B
0979     C *****
0980     C COMPUTE FLOW BETWEEN ADJACENT CELLS IN A SUBREGION OF THE GRID
0981     C *****
0982     C
0983     C SPECIFICATIONS:
0984     C -----
0985     C CHARACTER*16 TEXT(3)
0986     C DOUBLE PRECISION HNEW,HD
0987     C
0988     C DIMENSION HNEW(NCOL,NROW,NLAY), IBOUND(NCOL,NROW,NLAY),
0989     1     CR(NCOL,NROW,NLAY), CC(NCOL,NROW,NLAY),
0990     2     CV(NCOL,NROW,NLAY), TOP(NCOL,NROW,NLAY),
0991     3     BUFF(NCOL,NROW,NLAY)
0992     C
0993     C COMMON /FLWCOM/LAYCON(200)
0994     C
0995     C DATA TEXT(1),TEXT(2),TEXT(3)                                AT 0061
0996     1 /'FLOW RIGHT FACE ','FLOW FRONT FACE ','FLOW LOWER FACE '/
0997     C -----
0998     C
0999     C1-----IF CELL-BY-CELL FLOWS WILL BE SAVED IN A FILE, SET FLAG IBD.
1000     C1-----RETURN IF FLOWS ARE NOT BEING SAVED OR RETURNED.
1001     C ZERO=0.                                                    AT 0061
1002     C IBD=0                                                       AT 0075
1003     C IF(IBCFCB.GT.0) IBD=ICBCFL                                  AT 007F
1004     C IF(IBD.EQ.0 .AND. IBDRET.EQ.0) RETURN                       AT 0096
1005     C
1006     C2-----SET THE SUBREGION EQUAL TO THE ENTIRE GRID IF VALUES ARE BEING
1007     C2-----SAVED IN A FILE.
1008     C IF(IBD.NE.0) THEN                                          AT 00AF
1009.01         K1=1                                                AT 00BC
1010.01         K2=NLAY                                             AT 00C6
1011.01         I1=1                                               AT 00D1
1012.01         I2=NROW                                            AT 00DB
1013.01         J1=1                                               AT 00E6
1014.01         J2=NCOL                                            AT 00F0
1015.01         END IF                                             AT 00FB
1016.01     C
1017.01     C3-----TEST FOR DIRECTION OF CALCULATION; IF NOT ACROSS COLUMNS, GO TO
1018.01     C3-----STEP 4. IF ONLY 1 COLUMN, RETURN.
1019         IF(IDIR.NE.1) GO TO 405                                AT 00FB
1020         IF(NCOL.EQ.1) RETURN                                    AT 0107
1021     C
1022     C3A-----CALCULATE FLOW ACROSS COLUMNS (THROUGH RIGHT FACE). IF NOT
1023     C3A-----SAVING IN A FILE, SET THE SUBREGION. CLEAR THE BUFFER.
1024         IF(IBD.EQ.0) THEN                                        AT 0113
1025.01             K1=IL1                                           AT 0120
1026.01             K2=IL2                                           AT 012B
1027.01             I1=IR1                                           AT 0136
1028.01             I2=IR2                                           AT 0141
1029.01             J1=IC1-1                                         AT 014C
1030.01             IF(J1.LT.1) J1=1                                  AT 0158
1031.01             J2=IC2                                           AT 016B
1032.01         END IF                                             AT 0176
1033         DO 310 K=K1,K2                                         AT 0176
1034.01         DO 310 I=I1,I2                                       AT 01AB
1035.02         DO 310 J=J1,J2                                       AT 01E0
1036.03             BUFF(J,I,K)=ZERO                                  AT 0215
1037.03     310 CONTINUE                                          AT 024B
1038.03     C
1039.03     C3B-----FOR EACH CELL CALCULATE FLOW THRU RIGHT FACE & STORE IN BUFFER.
1040         IF(J2.EQ.NCOL) J2=J2-1                                AT 0257

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1041          DO 400 K=K1,K2                                AT 026E
1042.01      DO 400 I=I1,I2                                AT 02A3
1043.02      DO 400 J=J1,J2                                AT 02D8
1044.03      IF(ICHFLG.EQ.0) THEN                          AT 030D
1045.04          IF((IBOUND(J,I,K).LE.0) .AND. (IBOUND(J+1,I,K).LE.0)) GO TO 400 AT 0319
1046.04      ELSE                                          AT 0357
1047.04          IF((IBOUND(J,I,K).EQ.0) .OR. (IBOUND(J+1,I,K).EQ.0)) GO TO 400 AT 035C
1048.04      END IF                                        AT 039E
1049.03      HDIFF=HNEW(J,I,K)-HNEW(J+1,I,K)              AT 039E
1050.03      BUFF(J,I,K)=HDIFF*CR(J,I,K)                  AT 03D3
1051.03      400 CONTINUE                                  AT 0407
1052.03      C
1053.03      C3C-----RECORD CONTENTS OF BUFFER AND RETURN.
1054          IF(IBD.EQ.1)                                  AT 0416
1055      1      CALL UBUDSV(KSTP,KPER,TEXT(1),IBCFCB,BUFF,NCOL,NROW,NLAY,IOUT)
1056          IF(IBD.EQ.2) CALL UBDSV1(KSTP,KPER,TEXT(1),IBCFCB,BUFF,NCOL,NROW, AT 0450
1057      1      NLAY,IOUT,DELT,PERTIM,TOTIM,IBOUND)
1058          RETURN                                          AT 0496
1059      C
1060      C4-----TEST FOR DIRECTION OF CALCULATION; IF NOT ACROSS ROWS, GO TO
1061      C4-----STEP 5. IF ONLY 1 ROW, RETURN.
1062          405 IF(IDIR.NE.2) GO TO 505                    AT 049B
1063          IF(NROW.EQ.1) RETURN                          AT 04A7
1064      C
1065      C4A-----CALCULATE FLOW ACROSS ROWS (THROUGH FRONT FACE). IF NOT SAVING
1066      C4A-----IN A FILE, SET THE SUBREGION. CLEAR THE BUFFER.
1067          IF(IBD.EQ.0) THEN                              AT 04B3
1068.01      K1=IL1                                         AT 04C0
1069.01      K2=IL2                                         AT 04CB
1070.01      I1=IR1-1                                       AT 04D6
1071.01      IF(I1.LT.1) I1=1                               AT 04E2
1072.01      I2=IR2                                         AT 04F5
1073.01      J1=IC1                                         AT 0500
1074.01      J2=IC2                                         AT 050B
1075.01      END IF                                         AT 0516
1076          DO 410 K=K1,K2                                AT 0516
1077.01      DO 410 I=I1,I2                                AT 054B
1078.02      DO 410 J=J1,J2                                AT 0580
1079.03      BUFF(J,I,K)=ZERO                              AT 05B5
1080.03      410 CONTINUE                                  AT 05EB
1081.03      C
1082.03      C4B-----FOR EACH CELL CALCULATE FLOW THRU FRONT FACE & STORE IN BUFFER.
1083          IF(I2.EQ.NROW) I2=I2-1                       AT 05F7
1084          DO 500 K=K1,K2                                AT 060E
1085.01      DO 500 I=I1,I2                                AT 0643
1086.02      DO 500 J=J1,J2                                AT 0678
1087.03      IF(ICHFLG.EQ.0) THEN                          AT 06AD
1088.04          IF((IBOUND(J,I,K).LE.0) .AND. (IBOUND(J,I+1,K).LE.0)) GO TO 500 AT 06B9
1089.04      ELSE                                          AT 0722
1090.04          IF((IBOUND(J,I,K).EQ.0) .OR. (IBOUND(J,I+1,K).EQ.0)) GO TO 500 AT 0727
1091.04      END IF                                        AT 0794
1092.03      HDIFF=HNEW(J,I,K)-HNEW(J,I+1,K)              AT 0794
1093.03      BUFF(J,I,K)=HDIFF*CC(J,I,K)                  AT 07EE
1094.03      500 CONTINUE                                  AT 0822
1095.03      C
1096.03      C4C-----RECORD CONTENTS OF BUFFER AND RETURN.
1097          IF(IBD.EQ.1)                                  AT 0831
1098      1      CALL UBUDSV(KSTP,KPER,TEXT(2),IBCFCB,BUFF,NCOL,NROW,NLAY,IOUT)
1099          IF(IBD.EQ.2) CALL UBDSV1(KSTP,KPER,TEXT(2),IBCFCB,BUFF,NCOL,NROW, AT 086B
1100      1      NLAY,IOUT,DELT,PERTIM,TOTIM,IBOUND)
1101          RETURN                                          AT 08B1
1102      C
1103      C5-----DIRECTION OF CALCULATION IS ACROSS LAYERS BY ELIMINATION. IF
1104      C5-----ONLY 1 LAYER, RETURN.
1105          505 IF(NLAY.EQ.1) RETURN                      AT 08B6
1106      C
1107      C5A-----CALCULATE FLOW ACROSS LAYERS (THROUGH LOWER FACE). IF NOT
1108      C5A-----SAVING IN A FILE, SET THE SUBREGION. CLEAR THE BUFFER.
1109          IF(IBD.EQ.0) THEN                              AT 08C2
1110.01      K1=IL1-1                                       AT 08CF
1111.01      IF(K1.LT.1) K1=1                               AT 08DB
1112.01      K2=IL2                                         AT 08EE
1113.01      I1=IR1                                         AT 08F9
1114.01      I2=IR2                                         AT 0904
1115.01      J1=IC1                                         AT 090F
1116.01      J2=IC2                                         AT 091A
1117.01      END IF                                        AT 0925
1118          DO 510 K=K1,K2                                AT 0925
1119.01      DO 510 I=I1,I2                                AT 095A
1120.02      DO 510 J=J1,J2                                AT 098F
1121.03      BUFF(J,I,K)=ZERO                              AT 09C4
1122.03      510 CONTINUE                                  AT 09FA

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1123.03 C
1124.03 C5B----FOR EACH CELL CALCULATE FLOW THRU LOWER FACE & STORE IN BUFFER.
1125     IF (K2.EQ.NLAY) K2=K2-1
1126     KT=0
1127     DO 600 K=1,K2
1128 C-Environment Agency (UK)-1.Variable hydraulic cond. w/depth (VKD)>>>>>
1129 c     IF (LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.2) KT=KT+1
1130.01     IF (LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.2 .or. laycon(k).eq.5) KT=KT+1
1131.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
1132.01     IF (K.LT.K1) GO TO 600
1133.01     DO 590 I=I1,I2
1134.02     DO 590 J=J1,J2
1135.03     IF (ICHFLG.EQ.0) THEN
1136.04         IF ((IBOUND(J,I,K).LE.0) .AND. (IBOUND(J,I,K+1).LE.0)) GO TO 590
1137.04     ELSE
1138.04         IF ((IBOUND(J,I,K).EQ.0) .OR. (IBOUND(J,I,K+1).EQ.0)) GO TO 590
1139.04     END IF
1140.03     HD=HNEW(J,I,K+1)
1141.03 C-Environment Agency (UK)-1.Variable hydraulic cond. w/depth (VKD)>>>>>
1142.03 c     IF (LAYCON(K+1).NE.3 .AND. LAYCON(K+1).NE.2) GO TO 580
1143.03     IF (LAYCON(K+1).NE.3 .AND. LAYCON(K+1).NE.2 .and. laycon(k+1).ne.5)
1144.03     1     GO TO 580
1145.03 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
1146.03     TMP=HD
1147.03     IF (TMP.LT.TOP(J,I,KT+1)) HD=TOP(J,I,KT+1)
1148.03     580 HDIFF=HNEW(J,I,K)-HD
1149.03     BUFF(J,I,K)=HDIFF*CV(J,I,K)
1150.03     590 CONTINUE
1151.01     600 CONTINUE
1152.01 C
1153.01 C5C----RECORD CONTENTS OF BUFFER AND RETURN.
1154     IF (IBD.EQ.1)
1155     1     CALL UBDSV(KSTP,KPER,TEXT(3),IBCFB,BUFF,NCOL,NROW,NLAY,IOUT)
1156     IF (IBD.EQ.2) CALL UBDSV1(KSTP,KPER,TEXT(3),IBCFB,BUFF,NCOL,NROW,
1157     1     NLAY,IOUT,DELT,PERTIM,TOTIM,IBOUND)
1158     RETURN
1159     END
1160 C-Environment Agency (UK)-2.Variable storage with depth (VSD)>>>>>>>>
1161 c     SUBROUTINE SBCF5S(VBNM,VBVL,MSUM,HNEW,IBOUND,HOLD,SC1,
1162 c     1     TOP,SC2,DELT,ISS,NCOL,NROW,NLAY,KSTP,KPER,IBCFB,
1163 c     2     ICBCFL,BUFF,IOUT,PERTIM,TOTIM)

1164     SUBROUTINE SBCF5S(VBNM,VBVL,MSUM,HNEW,IBOUND,HOLD,SC1,
1165     1     TOP,SC2,DELT,ISS,NCOL,NROW,NLAY,KSTP,KPER,IBCFB,
1166     2     ICBCFL,BUFF,IOUT,PERTIM,TOTIM,bot,vmid,vsgrad,vsmid)
1167 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
1168 C-----VERSION 1257 28JUNE1993 SBCF5S
1169 C *****
1170 C COMPUTE STORAGE BUDGET FLOW TERM FOR BCF.
1171 C *****
1172 C
1173 C SPECIFICATIONS:
1174 C -----
1175 C CHARACTER*16 VBNM(MSUM),TEXT
1176 C-Environment Agency (UK)-2.Variable storage with depth (VSD)>>>>>>>>
1177 c     DOUBLE PRECISION HNEW,STOIN,STOUT,SSTRG
1178     DOUBLE PRECISION HNEW,STOIN,STOUT,SSTRG,htmp,vm,vsm,vsg,esm,bt,
1179     1     stmp,sold,snew,scof,rho1,rho2,tp
1180 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
1181 C
1182     DIMENSION HNEW(NCOL,NROW,NLAY), IBOUND(NCOL,NROW,NLAY),
1183     1     HOLD(NCOL,NROW,NLAY), SC1(NCOL,NROW,NLAY), VBVL(4,MSUM),
1184     2     SC2(NCOL,NROW,NLAY), TOP(NCOL,NROW,NLAY), BUFF(NCOL,NROW,NLAY)
1185 C-Environment Agency (UK)-2.Variable storage with depth (VSD)>>>>>>>>
1186     dimension bot(ncol,nrow,nlay), vmid(ncol,nrow,nlay),
1187     1     vsgrad(ncol,nrow,nlay), vsmid(ncol,nrow,nlay),
1188     2     vsmid(ncol,nrow,nlay)
1189 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
1190 C
1191     COMMON /FLWCOM/LAYCON(200)
1192 C
1193     DATA TEXT /'          STORAGE'/
1194 C -----
1195 C
1196 C1-----RETURN IF STEADY STATE.
1197     IF (ISS.NE.0) RETURN
1198 C
1199 C2-----INITIALIZE BUDGET ACCUMULATORS AND 1/DELT.
1200     ZERO=0.
1201     STOIN=ZERO

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1284.05      stmp = rho2*(htmp-bt)                                AT 08C7
1285.05      else                                              AT 08E0
1286.05      stmp = rho2*(tp-bt) + rho1*(htmp-tp)              AT 08E5
1287.05      endif                                              AT 0912
1288.05      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
1289.04      elseif((laycon(k).eq.5.and.htmp.le.tp).or.laycon(k).eq.4)then AT 0912
1290.04      if(htmp.le.esm)then                                  AT 0955
1291.05      stmp = rho2*(htmp-bt) + (rho2*vsg*(htmp-vm)**2)/2 AT 096B
1292.05      else                                              AT 09A8
1293.05      stmp = rho2*(esm-bt) + (rho2*vsg*(esm-vm)**2)/2 + AT 09AD
1294.05      1 (htmp-esm)*vsm*rho2
1295.05      endif                                              AT 0A04
1296.04      else                                              AT 0A04
1297.04      if(tp.le.esm)then                                  AT 0A09
1298.05      stmp = rho2*(tp-bt) + (rho2*vsg*(tp-vm)**2)/2 + rho1*(htmp-tp) AT 0A1F
1299.05      else                                              AT 0A70
1300.05      stmp = rho2*(esm-bt) + (rho2*vsg*(esm-vm)**2)/2 + AT 0A75
1301.05      1 (tp-esm)*vsm*rho2 + rho1*(htmp-tp)
1302.05      endif                                              AT 0AE0
1303.04      endif                                              AT 0AE0
1304.04      c
1305.04      c7c3---Find Storage At End Of Time Step
1306.03      if(itmp.eq.1)then                                  AT 0AE0
1307.04      sold=stmp                                          AT 0AED
1308.04      htmp=hnew(j,i,k)                                    AT 0B05
1309.04      itmp=0                                             AT 0B42
1310.04      goto 420                                          AT 0B4C
1311.04      endif                                              AT 0B51
1312.03      snew=stmp                                          AT 0B51
1313.03      c
1314.03      c7c4---Add Storage Terms To RHS and HCOF.
1315.03      strg = sold - snew                                  AT 0B69
1316.03      c
1317.03      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
1318.03      C
1319.03      C8-----STORE CELL-BY-CELL FLOW IN BUFFER AND ADD TO ACCUMULATORS.
1320.03      288 BUFF(J,I,K)=STRG                                AT 0B7C
1321.03      SSTRG=STRG                                          AT 0BB9
1322.03      IF(STRG) 292,300,294                                AT 0BD1
1323.03      292 STOUT=STOUT-SSTRG                              AT 0BF1
1324.03      GO TO 300                                          AT 0C04
1325.03      294 STOIN=STOIN+SSTRG                              AT 0C09
1326.03      C
1327.03      300 CONTINUE                                        AT 0C1C
1328.03      C
1329.03      C9-----IF IBD FLAG IS SET RECORD THE CONTENTS OF THE BUFFER.
1330      IF(IBD.EQ.1) CALL UBUDSV(KSTP,KPER,TEXT,              AT 0C2B
1331      1 IBCFCB,BUFF,NCOL,NROW,NLAY,IOUT)
1332      IF(IBD.EQ.2) CALL UBDSV1(KSTP,KPER,TEXT,IBCFCB,      AT 0C63
1333      1 BUFF,NCOL,NROW,NLAY,IOUT,DELT,PERTIM,TOTIM,IBOUND)
1334      C
1335      C10-----ADD TOTAL RATES AND VOLUMES TO VBVL & PUT TITLE IN VBNM.
1336      SIN=STOIN                                              AT 0CA7
1337      SOUT=STOUT                                             AT 0CBF
1338      VBVL(1,MSUM)=VBVL(1,MSUM)+SIN*DELT                  AT 0CD7
1339      VBVL(2,MSUM)=VBVL(2,MSUM)+SOUT*DELT                  AT 0CF7
1340      VBVL(3,MSUM)=SIN                                       AT 0D10
1341      VBVL(4,MSUM)=SOUT                                       AT 0D2C
1342      VBNM(MSUM)=TEXT                                         AT 0D4B
1343      MSUM=MSUM+1                                             AT 0D67
1344      C
1345      C11---RETURN.
1346      RETURN                                                  AT 0D6C
1347      END                                                    AT 0D71
COMMENT - SCOF has not been used

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1348      SUBROUTINE SBCF5F(VBNM,VBVL,MSUM,HNEW,IBOUND,CR,CC,CV, TOP,DELT,
1349      1 NCOL,NROW,NLAY,KSTP,KPER,IBCFCB,BUFF,IOUT,ICBCFL,
1350      2 PERTIM,TOTIM,ICHFLG)
1351      C-----VERSION 1315 18DEC1992 SBCF5F
1352      C *****
1353      C COMPUTE FLOW FROM CONSTANT-HEAD CELLS
1354      C *****
1355      C
1356      C SPECIFICATIONS:
1357      C -----
1358      C CHARACTER*16 VBNM(MSUM),TEXT
1359      C DOUBLE PRECISION HNEW,HD,CHIN,CHOUT,XX1,XX2,XX3,XX4,XX5,XX6
1360      C
1361      C DIMENSION HNEW(NCOL,NROW,NLAY), IBOUND(NCOL,NROW,NLAY),

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1362      1      CR(NCOL,NROW,NLAY), CC(NCOL,NROW,NLAY),
1363      2      CV(NCOL,NROW,NLAY), VBVL(4,MSUM),
1364      3      TOP(NCOL,NROW,NLAY),BUFF(NCOL,NROW,NLAY)
1365      C
1366      COMMON /FLWCOM/LAYCON(200)
1367      C
1368      DATA TEXT /'  CONSTANT HEAD'/
1369      C -----
1370      C
1371      C1-----SET IBD TO INDICATE IF CELL-BY-CELL BUDGET VALUES WILL BE SAVED.
1372      IBD=0
1373      IF(IBCFCB.LT.0 .AND. ICBCFL.NE.0) IBD=-1
1374      IF(IBCFCB.GT.0) IBD=ICBCFL
1375      C
1376      C2-----CLEAR BUDGET ACCUMULATORS.
1377      ZERO=0.
1378      CHIN=ZERO
1379      CHOUT=ZERO
1380      IBDLBL=0
1381      C
1382      C3-----CLEAR BUFFER.
1383      DO 5 K=1,NLAY
1384.01      DO 5 I=1,NROW
1385.02      DO 5 J=1,NCOL
1386.03      BUFF(J,I,K)=ZERO
1387.03      5      CONTINUE
1388.03      C
1389.03      C3A-----IF SAVING CELL-BY-CELL FLOW IN A LIST, COUNT CONSTANT-HEAD
1390.03      C3A-----CELLS AND WRITE HEADER RECORDS.
1391      IF(IBD.EQ.2) THEN
1392.01      NCH=0
1393.01      DO 7 K=1,NLAY
1394.02      DO 7 I=1,NROW
1395.03      DO 7 J=1,NCOL
1396.04      IF(IBOUND(J,I,K).LT.0) NCH=NCH+1
1397.04      7      CONTINUE
1398.01      CALL UBDSV2(KSTP,KPER,TEXT,IBCFCB,NCOL,NROW,NLAY,
1399.01      1      NCH,IOUT,DELT,PERTIM,TOTIM,IBOUND)
1400.01      END IF
1401.01      C
1402.01      C4-----LOOP THROUGH EACH CELL AND CALCULATE FLOW INTO MODEL FROM EACH
1403.01      C4-----CONSTANT-HEAD CELL.
1404      KT=0
1405      DO 200 K=1,NLAY
1406.01      LC=LAYCON(K)
1407.01      C-Environment Agency (UK)-2.Variable storage with depth (VSD)>>>>>>>>>
1408.01      c      IF(LC.EQ.3 .OR. LC.EQ.2) KT=KT+1
1409.01      IF(LC.EQ.3 .OR. LC.EQ.2 .or. lc.eq.5) KT=KT+1
1410.01      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<<
1411.01      DO 200 I=1,NROW
1412.02      DO 200 J=1,NCOL
1413.02      C
1414.02      C5-----IF CELL IS NOT CONSTANT HEAD SKIP IT & GO ON TO NEXT CELL.
1415.03      IF (IBOUND(J,I,K).GE.0)GO TO 200
1416.03      C
1417.03      C6-----CLEAR VALUES FOR FLOW RATE THROUGH EACH FACE OF CELL.
1418.03      X1=ZERO
1419.03      X2=ZERO
1420.03      X3=ZERO
1421.03      X4=ZERO
1422.03      X5=ZERO
1423.03      X6=ZERO
1424.03      C
1425.03      C7-----CALCULATE FLOW THROUGH THE LEFT FACE.
1426.03      C7-----COMMENTS A-C APPEAR ONLY IN THE SECTION HEADED BY COMMENT 7,
1427.03      C7-----BUT THEY APPLY IN A SIMILAR MANNER TO SECTIONS 8-12.
1428.03      C
1429.03      C7A-----IF THERE IS NO FLOW TO CALCULATE THROUGH THIS FACE, THEN GO ON
1430.03      C7A-----TO NEXT FACE. NO FLOW OCCURS AT THE EDGE OF THE GRID, TO AN
1431.03      C7A-----ADJACENT NO-FLOW CELL, OR TO AN ADJACENT CONSTANT-HEAD CELL
1432.03      C7A-----WHEN ICHFLG IS 0.
1433.03      IF(J.EQ.1) GO TO 30
1434.03      IF(IBOUND(J-1,I,K).EQ.0) GO TO 30
1435.03      IF(ICHFLG.EQ.0 .AND. IBOUND(J-1,I,K).LT.0) GO TO 30
1436.03      C
1437.03      C7B-----CALCULATE FLOW THROUGH THIS FACE INTO THE ADJACENT CELL.
1438.03      HDIFF=HNEW(J,I,K)-HNEW(J-1,I,K)
1439.03      X1=HDIFF*CR(J-1,I,K)
1440.03      XX1=X1
1441.03      C
1442.03      C7C-----ACCUMULATE POSITIVE AND NEGATIVE FLOW.
1443.03      IF (X1) 10,30,20

```

1444.03	10	CHOUT=CHOUT-XX1		AT 055A
1445.03		GO TO 30		AT 056D
1446.03	20	CHIN=CHIN+XX1		AT 0572
1447.03		C		
1448.03	C8-----	CALCULATE FLOW THROUGH THE RIGHT FACE.		
1449.03	30	IF (J.EQ.NCOL) GO TO 60		AT 0585
1450.03		IF (IBOUND(J+1,I,K).EQ.0) GO TO 60		AT 0596
1451.03		IF (ICHFLG.EQ.0 .AND. IBOUND(J+1,I,K).LT.0) GO TO 60		AT 05C6
1452.03		HDIFF=HNEW(J,I,K)-HNEW(J+1,I,K)		AT 05FF
1453.03		X2=HDIFF*CR(J,I,K)		AT 0631
1454.03		XX2=X2		AT 0661
1455.03		IF (X2) 40,60,50		AT 0679
1456.03	40	CHOUT=CHOUT-XX2		AT 0693
1457.03		GO TO 60		AT 06A6
1458.03	50	CHIN=CHIN+XX2		AT 06AB
1459.03		C		
1460.03	C9-----	CALCULATE FLOW THROUGH THE BACK FACE.		
1461.03	60	IF (I.EQ.1) GO TO 90		AT 06BE
1462.03		IF (IBOUND(J,I-1,K).EQ.0) GO TO 90		AT 06CB
1463.03		IF (ICHFLG.EQ.0 .AND. IBOUND(J,I-1,K).LT.0) GO TO 90		AT 0702
1464.03		HDIFF=HNEW(J,I,K)-HNEW(J,I-1,K)		AT 0742
1465.03		X3=HDIFF*CC(J,I-1,K)		AT 0799
1466.03		XX3=X3		AT 07CC
1467.03		IF (X3) 70,90,80		AT 07E4
1468.03	70	CHOUT=CHOUT-XX3		AT 07FE
1469.03		GO TO 90		AT 0811
1470.03	80	CHIN=CHIN+XX3		AT 0816
1471.03		C		
1472.03	C10-----	CALCULATE FLOW THROUGH THE FRONT FACE.		
1473.03	90	IF (I.EQ.NROW) GO TO 120		AT 0829
1474.03		IF (IBOUND(J,I+1,K).EQ.0) GO TO 120		AT 083A
1475.03		IF (ICHFLG.EQ.0 .AND. IBOUND(J,I+1,K).LT.0) GO TO 120		AT 086B
1476.03		HDIFF=HNEW(J,I,K)-HNEW(J,I+1,K)		AT 08AB
1477.03		X4=HDIFF*CC(J,I,K)		AT 0902
1478.03		XX4=X4		AT 0932
1479.03		IF (X4) 100,120,110		AT 094A
1480.03	100	CHOUT=CHOUT-XX4		AT 0964
1481.03		GO TO 120		AT 0977
1482.03	110	CHIN=CHIN+XX4		AT 097C
1483.03		C		
1484.03	C11-----	CALCULATE FLOW THROUGH THE UPPER FACE.		
1485.03	120	IF (K.EQ.1) GO TO 150		AT 098F
1486.03		IF (IBOUND(J,I,K-1).EQ.0) GO TO 150		AT 099C
1487.03		IF (ICHFLG.EQ.0 .AND. IBOUND(J,I,K-1).LT.0) GO TO 150		AT 09D1
1488.03		HD=HNEW(J,I,K)		AT 0A0F
1489.03	C-Environment Agency (UK)-1.Variable hydraulic cond. w/depth (VKD)>>>>>			
1490.03	c	IF (LC.NE.3 .AND. LC.NE.2) GO TO 122		
1491.03		IF (LC.NE.3 .AND. LC.NE.2 .and. lc.ne.5) GO TO 122		AT 0A46
1492.03	C-Environment Agency (UK)-End of this section of modified code <<<<<<<<			
1493.03		TMP=HD		AT 0A6D
1494.03		IF (TMP.LT.TOP(J,I,KT)) HD=TOP(J,I,KT)		AT 0A85
1495.03	122	HDIFF=HD-HNEW(J,I,K-1)		AT 0AF6
1496.03		X5=HDIFF*CV(J,I,K-1)		AT 0B2B
1497.03		XX5=X5		AT 0B5C
1498.03		IF (X5) 130,150,140		AT 0B74
1499.03	130	CHOUT=CHOUT-XX5		AT 0B8E
1500.03		GO TO 150		AT 0BA1
1501.03	140	CHIN=CHIN+XX5		AT 0BA6
1502.03		C		
1503.03	C12-----	CALCULATE FLOW THROUGH THE LOWER FACE.		
1504.03	150	IF (K.EQ.NLAY) GO TO 180		AT 0BB9
1505.03		IF (IBOUND(J,I,K+1).EQ.0) GO TO 180		AT 0BCA
1506.03		IF (ICHFLG.EQ.0 .AND. IBOUND(J,I,K+1).LT.0) GO TO 180		AT 0BF9
1507.03		HD=HNEW(J,I,K+1)		AT 0C37
1508.03	C-Environment Agency (UK)-1.Variable hydraulic cond. w/depth (VKD)>>>>>			
1509.03	c	IF (LAYCON(K+1).NE.3 .AND. LAYCON(K+1).NE.2) GO TO 152		
1510.03		IF (LAYCON(K+1).NE.3 .AND. LAYCON(K+1).NE.2 .and. laycon(k+1).ne.5)		AT 0C6F
1511.03	1	GO TO 152		
1512.03	C-Environment Agency (UK)-End of this section of modified code <<<<<<<<			
1513.03		TMP=HD		AT 0C9F
1514.03		IF (TMP.LT.TOP(J,I,KT+1)) HD=TOP(J,I,KT+1)		AT 0CB7
1515.03	152	HDIFF=HNEW(J,I,K)-HD		AT 0D2A
1516.03		X6=HDIFF*CV(J,I,K)		AT 0D5E
1517.03		XX6=X6		AT 0D8E
1518.03		IF (X6) 160,180,170		AT 0DA6
1519.03	160	CHOUT=CHOUT-XX6		AT 0DC0
1520.03		GO TO 180		AT 0DD3
1521.03	170	CHIN=CHIN+XX6		AT 0DD8
1522.03		C		
1523.03	C13-----	SUM THE FLOWS THROUGH SIX FACES OF CONSTANT HEAD CELL, AND		
1524.03	C13-----	STORE SUM IN BUFFER.		
1525.03	180	RATE=X1+X2+X3+X4+X5+X6		AT 0DEB


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1932.01 C10----RETURN.
1933      RETURN
1934      END
1935      C-Environment Agency (UK)-0.General change to enable new options>>>>>>>
1936      c      SUBROUTINE SBCF5N(HNEW, IBOUND, SC1, SC2, CR, CC, CV, HY, TRPY, DELR, DELC,
1937      c      1      ISS, NCOL, NROW, NLAY, IOUT, WETDRY, IWDFLG, CVWD)
COMMENT - HDA has not been used

1938      SUBROUTINE SBCF5N(HNEW, IBOUND, SC1, SC2, CR, CC, CV, HY, TRPY, DELR, DELC,
1939      1      ISS, NCOL, NROW, NLAY, IOUT, WETDRY, IWDFLG, CVWD, itrpy, vkgrad, vkmax,
1940      2      vsgrad, vsmax)
1941      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
1942      C
1943      C-----VERSION 1456 29JUNE1993 SBCF5N
1944      C      *****
1945      C      INITIALIZE AND CHECK BCF DATA
1946      C      *****
1947      C
1948      C      SPECIFICATIONS:
1949      C      -----
1950      C
1951      DOUBLE PRECISION HNEW,HCNV
1952      C
1953      C-Environment Agency (UK)-0.General change to enable new options>>>>>>>
1954      c      DIMENSION HNEW(NCOL, NROW, NLAY), IBOUND(NCOL, NROW, NLAY)
1955      c      1      , SC1(NCOL, NROW, NLAY), CR(NCOL, NROW, NLAY)
1956      c      2      , CC(NCOL, NROW, NLAY), CV(NCOL, NROW, NLAY)
1957      c      3      , HY(NCOL, NROW, NLAY), TRPY(NLAY), DELR(NCOL), DELC(NROW)
1958      c      4      , SC2(NCOL, NROW, NLAY), WETDRY(NCOL, NROW, NLAY)
1959      c      5      , CVWD(NCOL, NROW, NLAY)
1960      DIMENSION HNEW(NCOL, NROW, NLAY), IBOUND(NCOL, NROW, NLAY)
1961      1      , SC1(NCOL, NROW, NLAY), CR(NCOL, NROW, NLAY)
1962      2      , CC(NCOL, NROW, NLAY), CV(NCOL, NROW, NLAY)
1963      3      , HY(NCOL, NROW, NLAY), TRPY(ncol, nrow, nlay), DELR(NCOL), DELC(NROW)
1964      4      , SC2(NCOL, NROW, NLAY), WETDRY(NCOL, NROW, NLAY)
1965      5      , CVWD(NCOL, NROW, NLAY), vkgrad(ncol, nrow, nlay)
1966      6      , vkmax(ncol, nrow, nlay), vsgrad(ncol, nrow, nlay)
1967      7      , vsmax(ncol, nrow, nlay)
1968      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
1969      C
1970      COMMON /FLWCOM/LAYCON(200)
1971      COMMON /FLWAVG/LAYAVG(200)
1972      C      -----
1973      C
1974      C1-----MULTIPLY VERTICAL LEAKANCE BY AREA TO MAKE CONDUCTANCE.
1975      ZERO=0.
1976      IF(NLAY.EQ.1) GO TO 20
1977      K1=NLAY-1
1978      DO 10 K=1, K1
1979.01      DO 10 I=1, NROW
1980.02      DO 10 J=1, NCOL
1981.03      CV(J, I, K)=CV(J, I, K)*DELR(J)*DELC(I)
1982.03      10 CONTINUE
1983.03      C
1984.03      C2-----IF WETTING CAPABILITY IS ACTIVATED, SAVE CV IN CVWD FOR USE WHEN
1985.03      C2-----WETTING CELLS.
1986      IF(IWDFLG.EQ.0) GO TO 20
1987      DO 15 K=1, K1
1988.01      DO 15 I=1, NROW
1989.02      DO 15 J=1, NCOL
1990.03      CVWD(J, I, K)=CV(J, I, K)
1991.03      15 CONTINUE
1992.03      C
1993.03      C3-----IF IBOUND=0, SET CV=0 AND CC=0.
1994      DO 30 K=1, NLAY
1995.01      DO 30 I=1, NROW
1996.02      DO 30 J=1, NCOL
1997.03      IF(IBOUND(J, I, K).NE.0) GO TO 30
1998.03      IF(K.NE.NLAY) CV(J, I, K)=ZERO
1999.03      IF(K.NE.1) CV(J, I, K-1)=ZERO
2000.03      CC(J, I, K)=ZERO
2001.03      30 CONTINUE
2002.03      C
2003.03      C4-----INSURE THAT EACH ACTIVE CELL HAS AT LEAST ONE NON-ZERO
2004.03      C4-----TRANSMISSIVE PARAMETER.
2005      HCNV=888.88
2006      KB=0
2007      DO 60 K=1, NLAY
2008      C-Environment Agency (UK)-1.Variable hydraulic cond. w/depth (VKD)>>>>>
2009      c      IF(LAYCON(K).EQ.1 .OR. LAYCON(K).EQ.3) GO TO 50

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AT 2B3F
AT 2B44

AT 0061
AT 0075
AT 007E
AT 0085
AT 00AD
AT 00DA
AT 0107
AT 0143

AT 014F
AT 015B
AT 0189
AT 01B6
AT 01E3
AT 0215

AT 021E
AT 024B
AT 0278
AT 02A5
AT 02D5
AT 0315
AT 035A
AT 0391

AT 03A0
AT 03B4
AT 03BE


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2611 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
2612
2613 C-Environment Agency (UK)-3.Auto-conversion for steady state VKD>>>>>>>>
2614 c-----based on SBAS50,bas5df,bas5al,bas5rp,bcf5al & bcf5rp

2615 subroutine bcf5vk (hnew,inunit,inbcf,inbas,ibcfout,
2616 1 inout,ibasout,ncol,nrow,nlay,ifrefm,fname,cunit,IXSEC,
2617 2 NPER,iout,IBOUND,HOLD,TRPY,DELR,DELC,SC1,CC,HY,BOT,CV,
2618 3 TOP,SC2,vkgrad,WETDRY,buffer,cr,vmid,vkmax)
2619 c
2620 c-----version 11march1999 bcf5vk
2621 c *****
2622 c-----Writes new BCF, BAS and NAME files for 2nd initial conditions
2623 c-----for VKD run. Initial heads from previous (specified T) run,
2624 c-----top and bottom elevations calculated from heads and upper and
2625 c-----lower zone thicknesses, ISS set to 1, return to start of sim.
2626 c *****
2627 c
2628 c specifications:
2629 c -----
2630 c
2631 CHARACTER*24 ANAME(20)
2632 CHARACTER*4 CUNIT
2633 CHARACTER*80 LINE,fname,fnam2
2634 CHARACTER*11 FMTARG
2635 CHARACTER*80 HEADNG(2)
2636 CHARACTER*80 LINE1,LINE2
2637 character*20 fmtin(15,200)
2638 character*10 atmp,ahdry,awetfct
2639 character*30 PERLENNSTPTSMULT
2640 c
2641 dimension buff(ncol,nrow,nlay),HOLD(NCOL,NROW,NLAY),
2642 1 vkgrad(ncol,nrow,nlay),WETDRY(NCOL,NROW,NLAY),
2643 2 SC2(NCOL,NROW,NLAY),TOP(NCOL,NROW,NLAY),BOT(NCOL,NROW,NLAY),
2644 3 SC1(NCOL,NROW,NLAY),HY(NCOL,NROW,NLAY),CC(NCOL,NROW,NLAY),
2645 4 CV(NCOL,NROW,NLAY),TRPY(ncol,nrow,nlay),cr(ncol,nrow,nlay),
2646 5 vmid(ncol,nrow,nlay),vkmax(ncol,nrow,nlay)
2647 c
2648 integer IBOUND(NCOL,NROW,NLAY)
2649 c
2650 DOUBLE PRECISION HNEW,hhnew
2651 c
2652 DIMENSION HNEW(NCOL,NROW,NLAY),DELR(NCOL),DELC(NROW)
2653 common /flwcom/laycon(200)
2654 common /flwavg/layavg(200)
2655 c
2656 C -----
2657 c
2658 DATA ANAME(1) /' PRIMARY STORAGE COEF' / AT 0088
2659 DATA ANAME(2) /' TRANSMIS. ALONG ROWS' / AT 0088
2660 DATA ANAME(3) /' HYD. COND. ALONG ROWS' / AT 0088
2661 DATA ANAME(4) /' VERT HYD COND /THICKNESS' / AT 0088
2662 DATA ANAME(5) /' BOTTOM' / AT 0088
2663 DATA ANAME(6) /' TOP' / AT 0088
2664 DATA ANAME(7) /' SECONDARY STORAGE COEF' / AT 0088
2665 DATA ANAME(8) /' COLUMN TO ROW ANISOTROPY' / AT 0088
2666 DATA ANAME(9) /' DELR' / AT 0088
2667 DATA ANAME(10) /' DELC' / AT 0088
2668 DATA ANAME(11) /' WETDRY PARAMETER' / AT 0088
2669 data aname(12) /' HYD COND GRADIENT FACTOR' / AT 0088
2670 data aname(13) /' BOUNDARY ARRAY' / AT 0088
2671 data aname(14) /' STARTING HEADS' / AT 0088
2672 data aname(15) /' TRANSMIS. ALONG COLUMNS' / AT 0088
2673 data aname(16) /' HYD. COND. ALONG COLUMNS' / AT 0088
2674 data aname(17) /' ELEVATION OF CHANGE IN K' / AT 0088
2675 data aname(18) /' MAXIMUM HYD COND FACTOR' / AT 0088
2676 data aname(19) /' THICKNESS OF UPPER ZONE' / AT 0088
2677 DATA ANAME(20) /' THICKNESS OF LOWER ZONE' / AT 0088
2678 c
2679 C -----
2680 C
2681 C-----
2682 C1-----OPEN OLD AND NEW NAME FILES-----
2683 C1----- (CODE BASED ON SUBROUTINE 'SBAS50' IN BAS5.FOR) -----
2684 C-----
2685 OPEN(UNIT=inunit,FILE=FNAM2,STATUS='OLD') AT 0088
2686 lloc=1 AT 00BE
2687 call urword(fname,lloc,istart,istop,0,n,r,iout,inunit) AT 00C8
2688 fnam2=fname AT 010A
2689 fnam2(istop:istop)='2' AT 011C

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2690          OPEN(UNIT=inout,FILE=FNAM2)                                AT 012A
2691          write(iout,33)fnam2                                         AT 0154
2692 33        format(1x,/1x,'CREATING NEW NAME FILE: ',a)                AT 0194
2693          ierr=0                                                       AT 01D1
2694  C
2695  C1a-----READ A LINE; IGNORE BLANK LINES
2696 10        READ(INUNIT,'(A)',END=1000) LINE                            AT 01DB
2697          IF(LINE.EQ.' '.or.LINE(1:1).EQ. '#') then                    AT 023F
2698.01          write(inout,'(A)')line                                    AT 0261
2699.01          GO TO 10                                                 AT 02B9
2700.01          END IF                                                  AT 02BE
2701.01  C
2702.01  C1b-----DECODE THE FILE TYPE.
2703          LLOC=1                                                       AT 02BE
2704          CALL URWORD(LINE,LLOC,ITYP1,ITYP2,1,N,R,IOUT,INUNIT)         AT 02C8
2705          CALL URWORD(LINE,LLOC,ISTART,ISTOP,2,IU,R,IOUT,INUNIT)       AT 030E
2706          CALL URWORD(LINE,LLOC,INAM1,INAM2,0,N,R,IOUT,INUNIT)         AT 0354
2707  c
2708  C1c-----IF TYPE IS LIST, DATA OR BINARY, rename output files
2709          IF(LINE(ITYP1:ITYP2).EQ.'LIST'.or.line(ityp1:ityp2).eq.'DATA'.or. AT 039A
2710          1 line(ityp1:ityp2).eq.'DATA(BINARY)') then
2711.01 111      call urword(line,lloc,istart,istop,0,n,r,iout,inunit)     AT 0424
2712.01          if(line(istop:istop).eq.'>')then                       AT 046A
2713.02          call urword(line,lloc,istart,istop,0,n,r,iout,inunit)   AT 047E
2714.02          line1=line(istart:80)                                    AT 04C4
2715.02          write(line(inam1:80),'(a)')line1                        AT 04EE
2716.02          elseif(line(istart:istop).eq.'DIRECT')then              AT 0560
2717.02          call urword(line,lloc,istart,istop,2,irecl,r,iout,inunit) AT 0597
2718.02          goto 111                                                 AT 05DD
2719.02          elseif(line(ityp1:ityp2).ne.'DATA')then                 AT 05E2
2720.02          line(inam2:inam2)='2'                                    AT 0614
2721.02          endif                                                    AT 0622
2722.01          endif                                                  AT 0622
2723.01  c
2724.01  C1d-----IF TYPE IS BCF OR BAS, CREATE NEW BCF & BAS FILES (BC2 & BA2)
2725          if(line(ityp1:ityp2).eq.cunit.or.line(ityp1:ityp2).eq.'BAS')then AT 0622
2726.01          CALL URWORD(LINE,LLOC,ISTART,ISTOP,0,N,R,IOUT,INUNIT)     AT 0682
2727.01  c
2728.01  C1e-----CHANGE FILENAMES OF NEW BAS & BCF FILES
2729.01          IF(LINE(ityp1:ityp2).eq.cunit)then
2730.02          iu1=inbcf                                                 AT 06C8
2731.02          iu2=ibcfout                                              AT 06F9
2732.02          else                                                    AT 0707
2733.02          iu1=inbas                                                 AT 0715
2734.02          iu2=ibasout                                              AT 071A
2735.02          end if                                                  AT 0728
2736.01          IF(LINE(ISTOP:ISTOP).EQ.'>') THEN                       AT 0736
2737.02          OPEN(UNIT=IU1,FILE=LINE(INAM1:INAM2),FORM='FORMATTED',   AT 074A
2738.02          1 ACCESS='SEQUENTIAL')
2739.02          CALL URWORD(LINE,LLOC,ISTART,ISTOP,0,n,R,IOUT,INUNIT)     AT 07AA
2740.02          WRITE(IOUT,36) LINE(istart:istop),                       AT 07F0
2741.02          1 LINE(ITYP1:ITYP2),IU2
2742.02          OPEN(UNIT=IU2,FILE=LINE(ISTART:ISTOP),FORM='FORMATTED',   AT 0888
2743.02          1 ACCESS='SEQUENTIAL')
2744.02          line1=line(istart:istop)                                    AT 08E8
2745.02          write(line(inam1:80),'(a)')line1                        AT 0914
2746.02          ELSE                                                    AT 0986
2747.02          OPEN(UNIT=IU1,FILE=LINE(INAM1:INAM2),FORM='FORMATTED',   AT 098B
2748.02          1 ACCESS='SEQUENTIAL')
2749.02          line(inam2:inam2)='2'                                    AT 09EB
2750.02          WRITE(IOUT,36) LINE(INAM1:INAM2),                       AT 09F9
2751.02          1 LINE(ITYP1:ITYP2),IU2
2752.02 36        FORMAT(1X,/1X,'CREATING ',A,/                            AT 0A91
2753.02          1 1X,'FILE TYPE:',A,' UNIT',I4)
2754.02          OPEN(UNIT=IU2,FILE=LINE(INAM1:INAM2),FORM='FORMATTED',   AT 0AEE
2755.02          1 ACCESS='SEQUENTIAL')
2756.02          END IF                                                  AT 0B4E
2757.01          end if                                                  AT 0B4E
2758.01  c
2759.01  C1f-----WRITE FILENAMES IN NEW NAME FILE
2760          write(inout,'(A)')line                                       AT 0B4E
2761          GO TO 10                                                       AT 0BA6
2762          1000 CLOSE(UNIT=INUNIT)                                       AT 0BAB
2763          CLOSE(UNIT=INOUT)                                             AT 0BC3
2764          fname=fnam2                                                  AT 0BDB
2765  C -----
2766  c -----
2767  C-----
2768  C2-----READ OLD BAS FILE, WRITE NEW (BA2) FILE-----
2769  C2----- (CODE BASED ON BAS5DF, BAS5AL & BAS5RP)
2770  C-----
2771  c -----

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2772 C2a-----READ AND PRINT A HEADING.
2773     READ(INBAS,'(A)') HEADNG(1) AT OBED
2774     READ(INBAS,'(A)') HEADNG(2) AT OC45
2775     WRITE(IBASOUT,'(A)') HEADNG(1) AT OC9D
2776     WRITE(IBASOUT,'(A)') HEADNG(2) AT OCF5
2777 C
2778 C2b-----READ LINE SPECIFYING NUMBER OF LAYERS,ROWS,COLUMNS,STRESS
2779 C2b-----PERIODS AND UNITS OF TIME CODE, BUT DON'T DECODE.
2780     READ(INBAS,'(A)') LINE1 AT OD4D
2781     READ(INBAS,'(A)') LINE2 AT ODA5
2782     WRITE(IBASOUT,'(A)') LINE1 AT ODFD
2783     WRITE(IBASOUT,'(A)') LINE2 AT OE55
2784 c
2785 C2c-----READ & PRINT FLAG IAPART (RHS & BUFFER SHARE SPACE?) AND
2786 C2c-----FLAG ISTRT (SHOULD STARTING HEADS BE KEPT FOR DRAWDOWN?).
2787     IF(IFREFM.EQ.0) THEN AT OBAD
2788.01     READ(INBAS,'(2I10)') IAPART,ISTRT AT OBE9
2789.01     WRITE(IBASOUT,'(2I10)') IAPART,ISTRT AT OF1F
2790.01     ELSE AT OF85
2791.01     READ(INBAS,*) IAPART,ISTRT AT OF8A
2792.01     WRITE(IBASOUT,*) IAPART,ISTRT AT OFCF
2793.01     END IF AT 1014
2794.01 C
2795.01 C2d-----READ BOUNDARY ARRAY(BOUND) ONE LAYER AT A TIME.
2796     IF(IXSEC.EQ.0) THEN AT 1014
2797.01     DO 101 K=1,NLAY AT 1020
2798.02     KK=K AT 104D
2799.02     write(ibasout,64) inbas,k AT 1053
2800.02     CALL U2DINT(Ibound(1,1,kk),aname(13),nrow,ncol,0,INbas,iout) AT 10A3
2801.02     DO 102 I=1,nrow AT 10F9
2802.03     102 WRITE(IbasOUT,'(25I3)') (ibound(j,i,k),j=1,ncol) AT 1126
2803.02     101 CONTINUE AT 11D8
2804.01     ELSE AT 11DD
2805.01     CALL U2DINT(IBOUND(1,1,1),ANAME(13),NLAY,NCOL,-1,INBAS,IOUT) AT 11E2
2806.01     write(ibasout,63) inbas AT 1230
2807.01     DO 103 I=1,nlay AT 126C
2808.02     103 WRITE(IbasOUT,'(25I3)') (ibound(j,i,k),j=1,ncol) AT 1299
2809.01     END IF AT 134B
2810     64 format(i10,9x,'1(25I3)',22x,' 4 IBOUND Layer',i4) AT 134B
2811     63 format(i10,9x,'1(25I3)',22x,' 4 IBOUND') AT 1392
2812 C
2813 C2e-----READ AND PRINT HEAD VALUE TO BE PRINTED FOR NO-FLOW CELLS.
2814     IF(IFREFM.EQ.0) THEN AT 13CD
2815.01     READ(INBAS,'(a10)') aTMP AT 13D9
2816.01     WRITE(IBASOUT,'(a10)') aTMP AT 1431
2817.01     ELSE AT 1489
2818.01     READ(INBAS,*) TMP AT 148E
2819.01     WRITE(IBASOUT,*) TMP AT 14BF
2820.01     END IF AT 14F0
2821.01 C
2822.01 C2f-----READ INITIAL HEADS.
2823     IF(IXSEC.EQ.0) THEN AT 14F0
2824.01     DO 301 K=1,NLAY AT 14FC
2825.02     KK=K AT 1529
2826.02     CALL b12dri(fmtin(1,kk),HOLD(1,1,KK),NROW,NCOL,INBAS,IBASOUT,0, AT 152F
2827.02     1 0)
2828.02     301 CONTINUE AT 15A4
2829.01     ELSE AT 15A9
2830.01     CALL b12dri(fmtin(1,1),HOLD(1,1,1),NLAY,NCOL,INBAS,IBASOUT,0,0) AT 15AE
2831.01     END IF AT 1604
2832.01 c
2833.01 c2g-----Put heads calculated from specified transmissivity model into
2834.01 c2g-----new *.bas file as initial heads.
2835     IF(IXSEC.EQ.0) THEN AT 1604
2836.01     DO 302 K=1,NLAY AT 1610
2837.02     fmtin(1,k)='(10E23.16)' AT 163D
2838.02     write(ibasout,56) inbas,fmtin(1,k),aname(14),K AT 1661
2839.02     do 302 i=1,nrow AT 1702
2840.03     write(ibasout,fmtin(1,k)) (hnew(j,i,k),j=1,ncol) AT 172F
2841.03     302 CONTINUE AT 17ED
2842.01     ELSE AT 17F7
2843.01     write(ibasout,43) inbas,fmtin(1,1) AT 17FC
2844.01     do 303 i=1,nlay AT 1852
2845.02     write(ibasout,fmtin(1,1)) (hnew(j,i,k),j=1,ncol) AT 187F
2846.02     303 CONTINUE AT 1920
2847.01     56 format(i10,5x,'1.000',a20,8x,' 0',a24,' Layer',i4) AT 1925
2848.01     43 format(i10,5x,'1.000',a20,8x,'-1 STARTING HEADS') AT 196E
2849.01     END IF AT 19B5
2850.01 C
2851.01 C2h-----READ AND WRITE LENGTH OF STRESS PERIOD, NUMBER OF TIME STEPS AND
2852.01 C2h-----TIME STEP MULTIPLIER.
2853     DO 777 III=1,NPER AT 19B5

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2935.01 C3e2---READ TRANSMISSIVITY INTO ARRAY CC IF LAYER TYPE IS 0 OR 2.
2936.01 IF(LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.1 .or.laycon(k).eq.4 .or.
2937.01 1 laycon(k).eq.5) GO TO 100 AT 2298
2938.01 CALL b12dri(fmtin(6,k),CC(1,1,K),NROW,NCOL,INbcf,IOUT,0,0) AT 22D6
2939.01 if(itrpy.ne.2)goto 110 AT 234A
2940.01 do 14 i=1,nrow AT 2357
2941.02 do 14 j=1,ncol AT 2384
2942.03 cr(j,i,k)=cc(j,i,k) AT 23B4
2943.03 14 continue AT 23EC
2944.03 c
2945.03 c3e2i---READ Y-DIR TRANS IF TRPY=2.
2946.01 call b12dri(fmtin(2,k),cc(1,1,k),nrow,ncol,inbcf,iout,0,0) AT 23F3
2947.01 GO TO 110 AT 246D
2948.01 C
2949.01 C3e3---READ HYDRAULIC CONDUCTIVITY(HY) AND BOTTOM ELEVATION(BOT)
2950.01 C3e3---IF LAYER TYPE IS 1, 3, 4 or 5.
2951.01 100 CALL b12dri(fmtin(7,k),HY(1,1,KB),NROW,NCOL,INbcf,IOUT,0,0) AT 2472
2952.01 if(itrpy.ne.2)goto 105 AT 24EC
2953.01 c
2954.01 c3e3i---READ Y-DIR HYDRAULIC CONDUCTIVITY IF TRPY=2.
2955.01 call b12dri(fmtin(2,k),trpy(1,1,kb),nrow,ncol,inbcf,iout,0,0) AT 24F9
2956.01 105 CALL b12dri(fmtin(8,k),BOT(1,1,KB),NROW,NCOL,INbcf,IOUT,0,0) AT 2573
2957.01 C
2958.01 C3e4---READ VERTICAL HYCOND/THICK INTO ARRAY CV IF NOT BOTTOM LAYER;
2959.01 C3e4---MULTIPLIED BY CELL AREA TO CONVERT TO CONDUCTANCE LATER.
2960.01 110 IF(K.EQ.NLAY) GO TO 120 AT 25ED
2961.01 CALL b12dri(fmtin(9,k),CV(1,1,K),NROW,NCOL,INbcf,IOUT,0,0) AT 25FE
2962.01 C
2963.01 120 IF(LAYCON(K).NE.3.AND.LAYCON(K).NE.2.and.laycon(k).ne.5) GO TO 130 AT 2672
2964.01 C
2965.01 C3e5---READ TOP ELEVATION(TOP) IF LAYER TYPE IS 2, 3 or 5.
2966.01 CALL b12dri(fmtin(11,k),TOP(1,1,KT),NROW,NCOL,INbcf,IOUT,0,0) AT 26A2
2967.01 C
2968.01 C3e6---READ WETDRY CODES IF LAYER TYPE IS 1, 3, 4 or 5 AND WETTING
2969.01 C3e6---CAPABILITY HAS BEEN INVOKED (IWDFLG NOT 0).
2970.01 130 IF(LAYCON(K).NE.3 .AND. LAYCON(K).NE.1 .and. laycon(k).ne.4 .and.
2971.01 1 laycon(k).ne.5) GO TO 200 AT 271C
2972.01 IF(IWDFLG.EQ.0)GO TO 140 AT 275A
2973.01 CALL b12dri(fmtin(13,k),WETDRY(1,1,KB),NROW,NCOL,INbcf,IOUT,0,0) AT 2767
2974.01 c
2975.01 c3e7---read middle elevation into array VMID, hydraulic conductivity
2976.01 c3e7---gradient into array VKGRAD, and maximum hydraulic conductivity
2977.01 c3e7---into array VKMAX if layer type is 4 or 5.
2978.01 140 if(laycon(k).ne.4 .and. laycon(k).ne.5) go to 200 AT 27E1
2979.01 call b12dri(fmtin(14,k),vmid(1,1,kg),nrow,ncol,inbcf,iout,0,0) AT 2803
2980.01 fmtin(14,k)='(10E23.16)' AT 287D
2981.01 fmtin(7,k)='(10E23.16)' AT 28A9
2982.01 if(itrpy.eq.2.or.layavg(k).eq.40)fmtin(2,k)='(10E23.16)' AT 28D5
2983.01 call b12dri(fmtin(12,k),vkgrad(1,1,kg),nrow,ncol,inbcf,iout,0,0) AT 2922
2984.01 call b12dri(fmtin(15,k),vkmax(1,1,kg),nrow,ncol,inbcf,iout,0,0) AT 299C
2985.01 do 141 i=1,nrow AT 2A16
2986.02 do 141 j=1,ncol AT 2A43
2987.03 if(vkgrad(j,i,kg).le.0.0)then AT 2A73
2988.04 vkgrad(j,i,kg)=1.0 AT 2AB2
2989.04 vkmax(j,i,kg)=1.0 AT 2AE8
2990.04 endif AT 2B21
2991.03 141 continue AT 2B21
2992.03 c
2993.03 C-----
2994.03 C4-----CALCULATE NEW HYD COND, ANISOTROPY, AND MIDDLE ELEVATIONS IF
2995.03 C4-----LAYER TYPE IS 4 OR 5.
2996.03 C-----
2997.03 c
2998.03 c4a----CORRECT UPPER THICKNESSES IF THEY OVERLAP WITH THE BOTTOM
2999.01 150 if(laycon(k).eq.4.or.laycon(k).eq.5) then AT 2B2B
3000.02 do 42 j=1,ncol AT 2B4D
3001.03 do 42 i=1,nrow AT 2B7D
3002.04 if(laycon(k).eq.5.and.hnew(j,i,k).gt.top(j,i,kt)) then AT 2BAA
3003.05 if(vmid(j,i,kg).gt.top(j,i,kt)-bot(j,i,kb).and.ibound(j,i,k)
3004.05 1 .ne.0) then AT 2C29
3005.06 if(ierr.eq.0)then AT 2CFF
3006.07 ierr=1 AT 2DOC
3007.07 write(iout,*) AT 2D16
3008.07 write(iout,*)'TOP THICKNESSES REDUCED AT THE FOLLOWING L
3009.07 LOCATIONS:' AT 2D30
3010.07 write(iout,*)'Reduced FROM TO at LAYER,ROW,COL' AT 2D62
3011.07 write(iout,*)'-----' AT 2D94
3012.07 endif AT 2DC6
3013.06 write(iout,45)vmid(j,i,kg),top(j,i,kt)-bot(j,i,kb),k,i,j AT 2DC6
3014.06 45 format(2g12.4,'(,i3,',',i3,',',i3,')') AT 2EEA
3015.06 vmid(j,i,kg)=top(j,i,kt)-bot(j,i,kb) AT 2F2B
3016.06 endif AT 2FB3

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3017.05         else
3018.05         if (vmid(j,i,kg).gt.hnew(j,i,k)-bot(j,i,kb).and.ibound(j,i,k)
3019.05     1         .ne.0) then
3020.05             if(ierr.eq.0) then
3021.05                 ierr=1
3022.05                 write(iout,*)
3023.05                 write(iout,*) 'TOP THICKNESSES REDUCED AT THE FOLLOWING L
3024.05     LOCATIONS: '
3025.05                 write(iout,*) 'Reduced FROM TO at LAYER,ROW,COL'
3026.05                 write(iout,*) '-----'
3027.05                 endif
3028.05                 write(iout,45)vmid(j,i,kg),hnew(j,i,k)-bot(j,i,kb),k,i,j
3029.05                 vmid(j,i,kg)=hnew(j,i,k)-bot(j,i,kb)
3030.05             endif
3031.05         endif
3032.04     42     continue
3033.02     endif
3034.02     C
3035.02     C4B----LOOP THRU CELLS IN LAYER CALCULATING VKD PARAMETERS.
3036.01         do 44 j=1,ncol
3037.02         do 44 i=1,nrow
3038.03             if(ibound(j,i,k).eq.0)goto 44
3039.03         C
3040.03     C4C----INTERNODAL TRANSMISSIVITY OPTION.
3041.03         if(layavg(k).eq.40) then
3042.03         C
3043.03     C4C1----SET VARIABLES FOR X-DIR CALCULATIONS.
3044.04         jp=j+1
3045.04         ip=i+1
3046.04         if(j.eq.ncol)jp=j
3047.04         if(i.eq.nrow)ip=i
3048.04         bbot=(bot(j,i,kb)+bot(jp,i,kb))/2
3049.04         hhnew=(hnew(j,i,k)+hnew(jp,i,k))/2
3050.04         if(laycon(k).eq.3.or.laycon(k).eq.5) then
3051.05             ttop=(top(j,i,kt)+top(jp,i,kt))/2
3052.05             if(hhnew.gt.ttop)hhnew=ttop
3053.05         endif
3054.04         if(laycon(k).eq.4.or.laycon(k).eq.5) then
3055.05             vvmid=(vmid(j,i,kg)+vmid(jp,i,kg))/2
3056.05             vvkgrad=(vkgrad(j,i,kg)+vkgrad(jp,i,kg))/2
3057.05             vvkmax=(vkmax(j,i,kg)+vkmax(jp,i,kg))/2
3058.05             if(iss.eq.3) then
3059.06                 T=hy(j,i,kb)*(hhnew-bbot)
3060.06             else
3061.06                 T=hy(j,i,kb)
3062.06             endif
3063.06         C
3064.06     C4C2----CALCULATE X-DIR BASE HYDRAULIC CONDUCTIVITIES.
3065.05         if(vvmid.gt.(vvkmax-1.0)/vvkgrad) then
3066.06             buff(j,i,k)=T/(hhnew-bbot-(1.0/(2.0*vvkgrad))
3067.06     1             *(vvkmax-1.0)**2.0)+vvmid*(vvkmax-1.0)
3068.06             else
3069.06             buff(j,i,k)=T/((hhnew-vvmid-bbot)+vvmid
3070.06     1             *(1.0+0.5*vvkgrad*vvmid))
3071.06         endif
3072.06         C
3073.06     C4C3----CALCULATE X-DIR HYDRAULIC CONDUCTIVITIES (NOT USED)
3074.05         elseif(laycon(k).eq.1.or.laycon(k).eq.3) then
3075.05             buff(j,i,k)=hy(j,i,kb)/(hhnew-bbot)
3076.05         endif
3077.05         C
3078.05     C4C4----SET VARIABLES FOR Y-DIR CALCULATIONS.
3079.04         bbot=(bot(j,i,kb)+bot(j,ip,kb))/2
3080.04         hhnew=(hnew(j,i,k)+hnew(j,ip,k))/2
3081.04         if(laycon(k).eq.3.or.laycon(k).eq.5) then
3082.05             ttop=(top(j,i,kt)+top(j,ip,kt))/2
3083.05             if(hhnew.gt.ttop)hhnew=ttop
3084.05         endif
3085.04         if(laycon(k).eq.4.or.laycon(k).eq.5) then
3086.05             vvmid=(vmid(j,i,kg)+vmid(j,ip,kg))/2
3087.05             vvkgrad=(vkgrad(j,i,kg)+vkgrad(j,ip,kg))/2
3088.05             vvkmax=(vkmax(j,i,kg)+vkmax(j,ip,kg))/2
3089.05             if(itrpy.eq.2) then
3090.06                 T=trpy(j,i,kb)
3091.06             else
3092.06                 T=trpy(j,i,k)*hy(j,i,kb)/buff(j,i,k)
3093.06             endif
3094.05             if(iss.eq.3) T=T*(hhnew-bbot)
3095.05         C
3096.05     C4C5----CALCULATE Y-DIR BASE HYDRAULIC CONDUCTIVITIES.
3097.05         if(vvmid.gt.(vvkmax-1.0)/vvkgrad) then
3098.06             trpy(j,i,kb)=T/(hhnew-bbot-(1.0/(2.0*vvkgrad))

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3099.06      1      * (vvkmax - 1.0) ** 2.0 ) + vvmid * (vvkmax - 1.0) )
3100.06      else
3101.06      trpy(j,i,kb)= T / ((hhnew - vvmid - bbot) + vvmid *
3102.06      1      (1.0 + 0.5 * vvkgrad * vvmid))
3103.06      endif
3104.06      C
3105.06      C4C6----CALCULATE Y-DIR HYDRAULIC CONDUCTIVITIES (NOT USED)
3106.05      elseif(laycon(k).eq.1.or.laycon(k).eq.3)then
3107.05      if(itrpy.eq.2)then
3108.06      trpy(j,i,kb)=trpy(j,i,kb)/(hhnew - bbot)
3109.06      else
3110.06      trpy(j,i,k)=(trpy(j,i,k)*hy(j,i,kb)/(hhnew - bbot))/
3111.06      1      buff(j,i,k)
3112.06      end if
3113.05      endif
3114.04      hy(j,i,kb)=buff(j,i,k)
3115.04      C
3116.04      C4D-----BLOCK-CENTRED TRANSMISSIVITY OPTION.
3117.04      else
3118.04      C
3119.04      C4D1----CALCULATE BASE HYDRAULIC CONDUCTIVITIES.
3120.04      hhnew=hnew(j,i,k)
3121.04      if((laycon(k).eq.3.or.laycon(k).eq.5).and.
3122.04      1      hhnew.gt.top(j,i,kt))hhnew=top(j,i,kt)
3123.04      if(iss.eq.3)then
3124.05      T=hy(j,i,kb)*(hhnew-bot(j,i,kb))
3125.05      else
3126.05      T=hy(j,i,kb)
3127.05      endif
3128.04      if(laycon(k).eq.4.or.laycon(k).eq.5)then
3129.05      if(vmid(j,i,kg).gt.(vkmax(j,i,kg)-1.0)/vkgrad(j,i,kg))then
3130.06      hy(j,i,kb) = T / (hhnew-bot(j,i,kb) - (1.0
3131.06      1      / (2.0*vkgrad(j,i,kg)) * (vkmax(j,i,kg)-1.0)**2.0)
3132.06      2      +vmid(j,i,kg)*(vkmax(j,i,kg)-1.0))
3133.06      else
3134.06      hy(j,i,kb)= T / ((hhnew-vmid(j,i,kg)-bot(j,i,kb))+
3135.06      1      vmid(j,i,kg)*(1.0+0.5*vkgrad(j,i,kg)*vmid(j,i,kg)))
3136.06      endif
3137.06      C
3138.06      C4D2----CALCULATE HYDRAULIC CONDUCTIVITIES (NOT USED).
3139.05      elseif(laycon(k).eq.1.or.laycon(k).eq.3)then
3140.05      hy(j,i,kb)=hy(j,i,kb)/(hhnew-bot(j,i,kb))
3141.05      endif
3142.05      C
3143.05      C4D3----CALCULATE Y-DIR BASE HYDRAULIC CONDUCTIVITIES.
3144.04      if(itrpy.eq.2)then
3145.05      if(iss.eq.3)then
3146.06      T=trpy(j,i,kb)*(hhnew-bot(j,i,kb))
3147.06      else
3148.06      T=trpy(j,i,kb)
3149.06      endif
3150.05      if(laycon(k).eq.4.or.laycon(k).eq.5)then
3151.06      if(vmid(j,i,kg).gt.(vkmax(j,i,kg)-1.0)/vkgrad(j,i,kg))
3152.06      1      then
3153.07      trpy(j,i,kb)= T / (hhnew-bot(j,i,kb) - (1.0
3154.07      1      / (2.0*vkgrad(j,i,kg)) * (vkmax(j,i,kg)-1.0)**2.0)
3155.07      2      +vmid(j,i,kg)*(vkmax(j,i,kg)-1.0))
3156.07      else
3157.07      trpy(j,i,kb)= T / ((hhnew-vmid(j,i,kg)-
3158.07      1      bot(j,i,kb))+vmid(j,i,kg)*(1.0+0.5*vkgrad(j,i,kg)*
3159.07      2      vmid(j,i,kg)))
3160.07      endif
3161.07      C
3162.07      C4D4----CALCULATE Y-DIR HYDRAULIC CONDUCTIVITIES (NOT USED)
3163.06      elseif(laycon(k).eq.1.or.laycon(k).eq.3)then
3164.06      trpy(j,i,kb)=trpy(j,i,kb)/(hhnew-bot(j,i,kb))
3165.06      endif
3166.05      endif
3167.04      end if
3168.04      C
3169.04      C4E-----CALCULATE ELEVATION OF CHANGE IN K (MIDDLE ELEVATION, VMID).
3170.03      if(laycon(k).eq.4.or.laycon(k).eq.5)then
3171.04      if(laycon(k).eq.5.and.hnew(j,i,k).gt.top(j,i,kt))then
3172.05      vmid(j,i,kg)=top(j,i,kt)-vmid(j,i,kg)
3173.05      else
3174.05      vmid(j,i,kg)=hnew(j,i,k)-vmid(j,i,kg)
3175.05      endif
3176.04      endif
3177.03      44 continue
3178.03      C
3179.01      200 CONTINUE
3180.01      C

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3181.01 C-----
3182.01 C5-----WRITE NEW BCF FILE (BC2)
3183.01 c5----- (CODE BASED ON BCF5AL & BCF5RP)
3184.01 C-----
3185.01 c
3186.01 C5A-----CHANGE STEADY STATE FLAG BACK TO NORMAL VALUE (FROM 2 TO 1)
3187.01 C5A-----AND WRITE TOP TWO LINES OF NEW BCF FILE.
3188     ISS=1
3189     IF (IFREFM.EQ.0) THEN
3190.01         write(Ibcfout, '(2I10,a10,I10,a10,5I10)')
3191.01     1         ISS, IBCFCB, aHdry, IWDFlG, aWETFCT, IWETIT, IHDWET, itrpy
3192.01     2         , ihold, itrans
3193.01         write(Ibcfout, '(80I1)') (layavg(i)/10, LAYCon(I), I=1, NLAY)
3194.01     else
3195.01         write(Ibcfout, *) ISS, IBCFCB, Hdry, IWDFlG, WETFCT, IWETIT, IHDWET,
3196.01     1         itrpy, ihold, itrans
3197.01         write(Ibcfout, '(40(2i1,a1))') (layavg(i)/10, LAYCon(I), ' ',
3198.01     1         I=1, NLAY)
3199.01     end if
3200.01 C
3201.01 C5B-----WRITE ANISOTROPY RATIO
3202     if (itrpy.eq.0) then
3203.01         call SBCF5W(trpy(1,1,1), IBOUND, HNEW, NLAY, 1, NLAY, 0, INBCF,
3204.01     1         FMTIN(2,1), ANAME(8), IBCFOU, Hdry)
3205.01     elseif (itrpy.ne.2) then
3206.01         do 510 k=1, nlay
3207.02     510         call SBCF5W(trpy(1,1,K), IBOUND, HNEW, NCOL, NROW, NLAY, K, INBCF,
3208.02     1         FMTIN(2,k), ANAME(8), IBCFOU, Hdry)
3209.01     endif
3210.01 C
3211.01 c5C-----WRITE ROW SPACINGS (COLUMN WIDTHS)
3212     call SBCF5W(delr(1), IBOUND, HNEW, NCOL, 1, NLAY, 0, INBCF,
3213     1         FMTIN(3,1), ANAME(9), IBCFOU, Hdry)
3214     C
3215     C5D-----WRITE COLUMN SPACINGS (ROW HEIGHTS)
3216     call SBCF5W(delc(1), IBOUND, HNEW, Nrow, 1, NLAY, 0, INBCF,
3217     1         FMTIN(4,1), ANAME(10), IBCFOU, Hdry)
3218     C
3219     C5E-----WRITE ALL PARAMETERS FOR EACH LAYER.
3220     KT=0
3221     KB=0
3222     kg=0
3223     DO 400 K=1, NLAY
3224.01     KK=K
3225.01 C
3226.01 C5F-----FIND ADDRESS OF EACH LAYER IN THREE DIMENSION ARRAYS.
3227.01     IF (LAYCON(K).EQ.1 .OR. LAYCON(K).EQ.3 .or. laycon(k).eq.4 .or.
3228.01     1         laycon(k).eq.5) KB=KB+1
3229.01     IF (LAYCON(K).EQ.2 .OR. LAYCON(K).EQ.3 .or. laycon(k).eq.5) KT=KT+1
3230.01     if (laycon(k).eq.4 .or. laycon(k).eq.5) kg=kg+1
3231.01 C
3232.01 C5G-----write TRANSMISSIVITY INTO ARRAY CC IF LAYER TYPE IS 0 OR 2.
3233.01     IF (LAYCON(K).EQ.3 .OR. LAYCON(K).EQ.1 .or. laycon(k).eq.4 .or.
3234.01     1         laycon(k).eq.5) GO TO 300
3235.01     if (itrpy.ne.2) then
3236.02         call SBCF5W(cc(1,1,K), IBOUND, HNEW, NCOL, NROW, NLAY, K, INBCF,
3237.02     1         FMTIN(6,k), ANAME(2), IBCFOU, Hdry)
3238.02     else
3239.02         call SBCF5W(cr(1,1,K), IBOUND, HNEW, NCOL, NROW, NLAY, K, INBCF,
3240.02     1         FMTIN(6,k), ANAME(2), IBCFOU, Hdry)
3241.02         call SBCF5W(cc(1,1,K), IBOUND, HNEW, NCOL, NROW, NLAY, K, INBCF,
3242.02     1         FMTIN(2,k), ANAME(15), IBCFOU, Hdry)
3243.02     endif
3244.01     GO TO 310
3245.01 C
3246.01 C5H-----write HYDRAULIC CONDUCTIVITY (HY) AND BOTTOM ELEVATION (BOT)
3247.01 C5H-----IF LAYER TYPE IS 1, 3, 4 or 5.
3248.01     300 call SBCF5W(HY(1,1,KB), IBOUND, HNEW, NCOL, NROW, NLAY, K, INBCF,
3249.01     1         FMTIN(7,k), ANAME(3), IBCFOU, Hdry)
3250.01     if (itrpy.ne.2) goto 547
3251.01     call SBCF5W(trpy(1,1,KB), IBOUND, HNEW, NCOL, NROW, NLAY, K, INBCF,
3252.01     1         FMTIN(2,k), ANAME(16), IBCFOU, Hdry)
3253.01     547 call SBCF5W(bot(1,1,KB), IBOUND, HNEW, NCOL, NROW, NLAY, K, INBCF,
3254.01     1         FMTIN(8,k), ANAME(5), IBCFOU, Hdry)
3255.01 C
3256.01 C5I-----write VERTICAL HYCOND/THICK INTO ARRAY CV IF NOT BOTTOM LAYER;
3257.01 C5I-----MULTIPLIED BY CELL AREA TO CONVERT TO CONDUCTANCE LATER.
3258.01     310 IF (K.EQ.NLAY) GO TO 320
3259.01         call SBCF5W(CV(1,1,K), IBOUND, HNEW, NCOL, NROW, NLAY, K, INBCF,
3260.01     1         FMTIN(9,k), ANAME(4), IBCFOU, Hdry)
3261.01 C
3262.01     320 IF (LAYCON(K).NE.3.AND.LAYCON(K).NE.2.and.laycon(k).ne.5) GO TO 330

```

```

3263.01 C
3264.01 C5J-----write TOP ELEVATION(TOP) IF LAYER TYPE IS 2, 3 or 5.
3265.01 call SBCF5W(TOP(1,1,KT), IBOUND,HNEW,NCOL,NROW,NLAY,K, INBCF, AT 521F
3266.01 1 FMTIN(11,k), ANAME(6), IBCFOUT,HDRY)
3267.01 C
3268.01 C5K-----write WETDRY CODES IF LAYER TYPE IS 1, 3, 4 or 5 AND WETTING
3269.01 C5K-----CAPABILITY HAS BEEN INVOKED (IWDFLG NOT 0).
3270.01 330 IF(LAYCON(K).NE.3 .AND. LAYCON(K).NE.1 .and. laycon(k).ne.4 .and. AT 52B9
3271.01 1 laycon(k).ne.5)GO TO 400
3272.01 IF(IWDFLG.EQ.0)GO TO 340 AT 52F7
3273.01 call SBCF5W(WETDRY(1,1,KB), IBOUND,HNEW,NCOL,NROW,NLAY,K, INBCF, AT 5304
3274.01 1 FMTIN(13,k), ANAME(11), IBCFOUT,HDRY)
3275.01 c
3276.01 C5L-----WRITE HYDRAULIC CONDUCTIVITY GRADIENT FROM ARRAY VKGRAD,
3277.01 C5L-----MIDDLE ELEVATION FROM ARRAY VMID and maximum hyd cond IF LAYER
3278.01 C5L-----TYPE IS 4 OR 5.
3279.01 340 if(laycon(k).ne.4 .and. laycon(k).ne.5) go to 400 AT 539E
3280.01 call SBCF5W(VMID(1,1,KG), IBOUND,HNEW,NCOL,NROW,NLAY,K, INBCF, AT 53C0
3281.01 1 FMTIN(14,k), ANAME(17), IBCFOUT,HDRY)
3282.01 call SBCF5W(VKGRAD(1,1,KG), IBOUND,HNEW,NCOL,NROW,NLAY,K, INBCF, AT 545A
3283.01 1 FMTIN(12,k), ANAME(12), IBCFOUT,HDRY)
3284.01 call SBCF5W(VKMAX(1,1,KG), IBOUND,HNEW,NCOL,NROW,NLAY,K, INBCF, AT 54F4
3285.01 1 FMTIN(15,k), ANAME(18), IBCFOUT,HDRY)
3286.01 C
3287.01 C5M-----WRITE NEW UPPER THICKNESSES TO 1ST OUTPUT FILE IF THEY HAVE
3288.01 C5M-----BEEN CHANGED.
3289.01 if(ierr.eq.1)then AT 558E
3290.02 do i=1,nrow AT 559B
3291.03 do j=1,ncol AT 55C8
3292.04 if(laycon(k).eq.5.and.hnew(j,i,k).gt.top(j,i,kt))then AT 55F8
3293.05 buff(j,i,1)=top(j,i,kt)-vmid(j,i,kg) AT 5677
3294.05 else AT 56F5
3295.05 buff(j,i,1)=hnew(j,i,k)-vmid(j,i,kg) AT 56FA
3296.05 endif AT 577E
3297.04 enddo AT 577E
3298.03 enddo AT 5783
3299.02 WRITE(IOUT,94) ANAME(19),K AT 5788
3300.02 94 FORMAT(1X,///11X,A,' FOR LAYER',I4) AT 57DC
3301.02 call ulaprw(buff,aname(19),0,0,ncol,nrow,0,1,iout) AT 5811
3302.02 endif AT 5849
3303.02 C
3304.02 C5N-----WRITE LOWER THICKNESSES TO 1ST OUTPUT FILE.
3305.01 do i=1,nrow AT 5849
3306.02 do j=1,ncol AT 5876
3307.03 buff(j,i,1)=vmid(j,i,kg)-bot(j,i,kg) AT 58A6
3308.03 enddo AT 591B
3309.02 enddo AT 5920
3310.01 WRITE(IOUT,94) ANAME(20),K AT 5925
3311.01 call ulaprw(buff,aname(20),0,0,ncol,nrow,0,1,iout) AT 5979
3312.01 400 continue AT 59B1
3313.01 C
3314 close(unit=ibcfout) AT 59B6
3315 C
3316 C99-----RETURN
3317 RETURN AT 59CE
3318 END AT 59D3
3319 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
3320
3321
3322 C-Environment Agency (UK)-3.Auto-conversion for steady state VKD>>>>>>>>
3323 C-----BASED ON U2DINT, uldint & u2drel FROM UTL5.FOR
WARNING - Label 150 has not been referenced
COMMENT - FMTARG has not been used

```

```

3324 SUBROUTINE B12DRI(fmtin,A,II,JJ,IN,IOUT,iint,ip)
3325 C
3326 C-----VERSION 0001 11MAR1999 B12DRI
3327 C *****
3328 C ROUTINE TO INPUT 1 & 2-D real DATA MATRICES
3329 C A IS ARRAY TO INPUT
3330 C II IS NO. OF ROWS
3331 C JJ IS NO. OF COLS
3332 C IN IS INPUT UNIT
3333 C IOUT IS OUTPUT UNIT
3334 c iint is 1 for integer array(option removed),otherwise:real array
3335 c ip is set to 0 to dissable printing to file
3336 C *****
3337 C
3338 C SPECIFICATIONS:
3339 C -----

```

```

3340         DIMENSION A(JJ,II)
3341         CHARACTER*20 FMTIN
3342         CHARACTER*80 CNTRL
3343         character*80 fname
3344         data nunopn/99/
3345     C -----
3346     C
3347     C1-----READ ARRAY CONTROL RECORD AS CHARACTER DATA.
3348         READ(IN,'(A)') CNTRL
3349         if(ip.ne.0)WRITE(IOUT,'(A)') CNTRL
3350
3351     C
3352     C2-----LOOK FOR ALPHABETIC WORD THAT INDICATES THAT THE RECORD IS FREE
3353     C2-----FORMAT.  SET A FLAG SPECIFYING IF FREE FORMAT OR FIXED FORMAT.
3354         ICLOSE=0
3355         IFREE=1
3356         ICOL=1
3357         CALL URWORD(CNTRL,ICOL,ISTART,ISTOP,1,N,R,IOUT,IN)
3358         IF (CNTRL(ISTART:ISTOP).EQ.'CONSTANT') THEN
3359.01         locat=0
3360.01     ELSE IF (CNTRL(ISTART:ISTOP).EQ.'INTERNAL') THEN
3361.01         LOCAT=IN
3362.01     ELSE IF (CNTRL(ISTART:ISTOP).EQ.'EXTERNAL') THEN
3363.01         CALL URWORD(CNTRL,ICOL,ISTART,ISTOP,2,LOCAT,R,IOUT,IN)
3364.01     ELSE IF (CNTRL(ISTART:ISTOP).EQ.'OPEN/CLOSE') THEN
3365.01         CALL URWORD(CNTRL,ICOL,ISTART,ISTOP,0,N,R,IOUT,IN)
3366.01         FNAME=CNTRL(ISTART:ISTOP)
3367.01         LOCAT=NUNOPN
3368.01         OPEN(UNIT=LOCAT,FILE=FNAME)
3369.01         ICLOSE=1
3370.01     ELSE
3371.01     C
3372.01     C2A-----DID NOT FIND A RECOGNIZED WORD, SO NOT USING FREE FORMAT.
3373.01     C2A-----READ THE CONTROL RECORD THE ORIGINAL WAY.
3374.01         IFREE=0
3375.01         READ(CNTRL,1) LOCAT,CONST,FMTIN,IPRN
3376.01         1  FORMAT(I10,f10.0,A20,I10)
3377.01     END IF
3378.01     C
3379.01     C3-----FOR FREE FORMAT CONTROL RECORD, READ REMAINING FIELDS.
3380         IF(IFREE.NE.0) THEN
3381.01         CALL URWORD(CNTRL,ICOL,ISTART,ISTOP,3,N,CONST,IOUT,IN)
3382.01         IF(LOCAT.NE.0) THEN
3383.02         CALL URWORD(CNTRL,ICOL,ISTART,ISTOP,1,N,R,IOUT,IN)
3384.02         FMTIN=CNTRL(ISTART:ISTOP)
3385.02         IF(ICLOSE.NE.0) THEN
3386.03         IF(FMTIN.EQ.'(BINARY)') THEN
3387.04         OPEN(UNIT=LOCAT,FILE=FNAME,FORM='UNFORMATTED')
3388.04         ELSE
3389.04         OPEN(UNIT=LOCAT,FILE=FNAME)
3390.04         END IF
3391.03         END IF
3392.02         IF(LOCAT.GT.0 .AND. FMTIN.EQ.'BINARY') LOCAT=-LOCAT
3393.02         CALL URWORD(CNTRL,ICOL,ISTART,ISTOP,2,IPRN,R,IOUT,IN)
3394.02         END IF
3395.01     END IF
3396.01     C
3397.01     C4-----TEST LOCAT TO SEE HOW TO DEFINE ARRAY VALUES.
3398         IF(LOCAT) 200,50,90
3399     C
3400     C4A-----LOCAT=0; SET ALL ARRAY VALUES EQUAL TO CONST. RETURN.
3401         50 DO 80 I=1,II
3402.01         DO 80 J=1,JJ
3403.02         80  a(j,i)=const
3404         RETURN
3405     C
3406     C4B-----LOCAT>0; READ & WRITE FORMATTED RECORDS USING FORMAT FMTIN.
3407         90 DO 110 I=1,II
3408.01         IF(FMTIN.EQ.'(FREE)') THEN
3409.02         READ(LOCAT,*) (A(J,I),J=1,JJ)
3410.02         if(ip.ne.0)WRITE(IOUT,*) (A(J,I),J=1,JJ)
3411.02         ELSE
3412.02         READ(LOCAT,FMTIN) (A(J,I),J=1,JJ)
3413.02         if(ip.ne.0)WRITE(IOUT,FMTIN) (A(J,I),J=1,JJ)
3414.02         END IF
3415.01         110 CONTINUE
3416.01     C
3417         go to 300
3418     C
3419     C4C-----LOCAT<0; READ UNFORMATTED RECORD CONTAINING ARRAY VALUES.
3420         200 LOCAT=-LOCAT
3421         READ(LOCAT)

```



```

3422         READ(LOCAT) A                                     AT 08E6
3423         C
3424         C5-----IF CONST NOT ZERO THEN MULTIPLY ARRAY VALUES BY CONST.
3425         300 IF(ICLOSE.NE.0) CLOSE(UNIT=LOCAT)             AT 0913
3426         IF(CONST.EQ.0) GO TO 320                          AT 0939
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
3427         DO 310 I=1,II                                     AT 094F
3428.01      DO 310 J=1,JJ                                     AT 097C
3429.02      A(J,I)=A(J,I)*CONST                             AT 09A9
3430.02      310 CONTINUE                                    AT 09CA
3431.02     C
3432         320 RETURN                                        AT 09CE
3433         END                                             AT 09D3
3434         C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
3435
3436         C-Environment Agency (UK)-8.Output calculated transmissivities>>>>>>>>
3437         c-----based on subroutine sbas5h in bas package----
3438         C-Environment Agency (UK)-11.Output calc trans to binary file>>>>>>>>
3439         c      subroutine bcf5ot(cc,cr,BUFF,KSTP,KPER,NCOL,NROW,NLAY,IOUT,
3440         c      1 IXSEC,delc,delr,itrpy,trpy,ihedfm,cv)

3441         subroutine bcf5ot(cc,cr,BUFF,KSTP,KPER,NCOL,NROW,NLAY,IOUT,
3442         1 IXSEC,delc,delr,itrpy,trpy,ihedfm,cv,itrans,ioflg,CHEDFM,
3443         2 LBHDSV,IBOUND,PERTIM,TOTIM)
3444         C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
3445         C
3446         C-----VERSION 1647 18OCT1993 bcf5ot
3447         C *****
3448         C PRINT AND RECORD internodal transmissivities
3449         C *****
3450         C
3451         C SPECIFICATIONS:
3452         C -----
3453         CHARACTER*16 TEXT
3454         C-Environment Agency (UK)-11.Output calc trans to binary file>>>>>>>>
3455         c      DIMENSION cc(NCOL,NROW,NLAY),BUFF(NCOL,NROW,NLAY),
3456         c      1 cr(ncol,nrow,nlay),trpy(ncol,nrow,nlay),
3457         c      2 delc(nrow),delr(ncol),cv(ncol,nrow,nlay)
3458         DIMENSION cc(NCOL,NROW,NLAY),BUFF(NCOL,NROW,NLAY),
3459         1 cr(ncol,nrow,nlay),trpy(ncol,nrow,nlay),
3460         2 delc(nrow),delr(ncol),cv(ncol,nrow,nlay),
3461         3 ioflg(nlay,4),IBOUND(NCOL,NROW,NLAY)
3462         CHARACTER*20 CHEDFM
3463         C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
3464         C -----
3465         C
3466         DO 100 ITRAN=1,3                                     AT 0079
3467.01      if(itran.eq.1)text='X-DIR INTR-TRANS '           AT 0096
3468.01      if(itran.eq.2)text='Y-DIR INTR-TRANS '           AT 00B6
3469.01      if(itran.eq.3)text='Z-DIR INTR-COND. '           AT 00D6
3470.01
3471.01     C1-----FOR EACH LAYER put transmissivity in BUFF
3472.01      DO 59 K=1,NLAY                                     AT 00F6
3473.01     C
3474.01     C2-----Set temporary variables
3475.02      KL=K                                               AT 0123
3476.02      IF(IXSEC.NE.0) KL=1                               AT 0129
3477.02      if(itrpy.eq.0)yx=trpy(k,1,1)                     AT 013F
3478.02     C
3479.02     C3-----put transmissivity into BUFF FOR THE LAYER.
3480.02      DO 58 I=1,NROW                                     AT 0176
3481.03      DO 58 J=1,NCOL                                    AT 01A3
3482.04      if (itran.eq.1) then                               AT 01D0
3483.05          if (j.ne.ncol) then                           AT 01DD
3484.06              BUFF(J,I,K)=cr(J,I,K)*(delr(j+1)+delr(j))/(2*delc(i))
3485.06              else                                       AT 01E8
3486.06                  buff(j,i,k)=0                            AT 0233
3487.06              end if                                       AT 0238
3488.05          elseif(itran.eq.2)then                         AT 026B
3489.05              if (i.ne.nrow) then                          AT 027D
3490.06                  BUFF(J,I,K)=cc(J,I,K)*(delc(i+1)+delc(i))/(2*delr(j))
3491.06                  else                                       AT 028E
3492.06                      buff(j,i,k)=0                            AT 02D9
3493.06                  end if                                       AT 02DE
3494.05              else                                       AT 0311
3495.05                  if (k.ne.nlay) then                       AT 0311
3496.06                      BUFF(J,I,K)=cv(J,I,K)/(delc(i)*delr(j))
3497.06                      else                                       AT 0316
3498.06                          goto 100                            AT 0327
3499.06                      end if                                       AT 036E
3499.06                  end if                                       AT 0373
3499.06                  end if                                       AT 0378

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3500.05      end if
3501.04      58 CONTINUE
3502.02      59 CONTINUE
3503.02      C
3504.02      C4-----FOR EACH LAYER PRINT x- and y-dir internodal transmissivities.
3505.02      C-Environment Agency (UK)-11.Output calc trans to binary file>>>>>>>>>>>>
3506.01      if (itrans.le.0) goto 70
3507.01      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<<<<
3508.01      IF (IXSEC.EQ.0) THEN
3509.02          DO 69 K=1,NLAY
3510.03          KK=K
3511.03          if (ihedfm.lt.0) CALL ULAPRS (BUFF (1,1,K) ,TEXT ,KSTP ,KPER ,NCOL ,NROW ,
3512.03      1          KK , -ihedfm ,IOUT)
3513.03          if (ihedfm.ge.0) CALL ULAPRW (BUFF (1,1,K) ,TEXT ,KSTP ,KPER ,NCOL ,NROW ,
3514.03      1          KK , ihedfm ,IOUT)
3515.03      69 CONTINUE
3516.03      C
3517.03      C4A----PRINT transmissivities FOR CROSS SECTION (?).
3518.02      ELSE
3519.02          if (ihedfm.lt.0) CALL ULAPRS (BUFF ,TEXT ,KSTP ,KPER ,NCOL ,NLAY , -1 ,
3520.02      1          - ihedfm ,IOUT)
3521.02          if (ihedfm.ge.0) CALL ULAPRW (BUFF ,TEXT ,KSTP ,KPER ,NCOL ,NLAY , -1 ,
3522.02      1          ihedfm ,IOUT)
3523.02      END IF
3524.02      C-Environment Agency (UK)-11.Output calc trans to binary file>>>>>>>>>>>>
3525.02      C
3526.02      C5-----FOR EACH LAYER: DETERMINE IF HEAD SHOULD BE SAVED ON DISK.
3527.02      C5-----IF SO THEN CALL ULASAV OR ULASV2 TO SAVE HEAD.
3528.01      70 IFIRST=1
3529.01      IF (itrans.ge.0) GO TO 100
3530.01      IF (IXSEC.EQ.0) THEN
3531.02          DO 79 K=1,NLAY
3532.03          KK=K
3533.03          IF (IOFLG (K,3) .EQ.0) GO TO 79
3534.03          IF (IFIRST.EQ.1) WRITE (IOUT,74) text , -itrans ,KSTP ,KPER
3535.03      74 FORMAT (1X ,/1X ,a16 , ' WILL BE SAVED ON UNIT' ,I4 ,
3536.03      1          ' AT END OF TIME STEP' ,I3 , ' , STRESS PERIOD' ,I3)
3537.03          IFIRST=0
3538.03          IF (CHEDFM.EQ. ' ') THEN
3539.04          CALL ULASAV (BUFF (1,1,K) ,TEXT ,KSTP ,KPER ,PERTIM ,TOTIM ,NCOL ,
3540.04      1          NROW ,KK , -itrans)
3541.04          ELSE
3542.04          CALL ULASV2 (BUFF (1,1,K) ,TEXT ,KSTP ,KPER ,PERTIM ,TOTIM ,NCOL ,
3543.04      1          NROW ,KK , -itrans ,CHEDFM ,LBHDSV , IBOUND (1,1,K) )
3544.04          END IF
3545.03      79 CONTINUE
3546.03      C
3547.03      C5A----SAVE HEAD FOR CROSS SECTION.
3548.02      ELSE
3549.02          IF (IOFLG (1,3) .NE.0) THEN
3550.03          WRITE (IOUT,74) text , -itrans ,KSTP ,KPER
3551.03          IF (CHEDFM.EQ. ' ') THEN
3552.04          CALL ULASAV (BUFF ,TEXT ,KSTP ,KPER ,PERTIM ,TOTIM ,NCOL ,
3553.04      1          NLAY , -1 , -itrans)
3554.04          ELSE
3555.04          CALL ULASV2 (BUFF ,TEXT ,KSTP ,KPER ,PERTIM ,TOTIM ,NCOL ,
3556.04      1          NLAY , -1 , -itrans ,CHEDFM ,LBHDSV , IBOUND)
3557.04          END IF
3558.03          END IF
3559.02          END IF
3560.02      C
3561.01      100 continue
3562.01      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<<<<
3563.01      C
3564.01      c5-----return
3565          return
3566          end
3567      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<<<<
3568
3569      C-Environment Agency (UK)-3.Auto-conversion for steady state VKD>>>>>>>>>>>>

3570          subroutine SBCF5W (A , IBOUND , HNEW , NCOL , NROW , NLAY , K , INBCF , FMT , ANAME ,
3571      1          IBCFOUT , HDRY)
3572      C
3573      C-----VERSION 0001 15FEB2001 SBCF5W
3574      C *****
3575      C WRITES ARRAYS TO SECOND BCF FILE
3576      C *****
3577      C
3578      C SPECIFICATIONS:

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3579      C      -----
3580      double precision HNEW
3581      dimension A (NCOL,NROW) , IBOUND (NCOL,NROW,NLAY) , HNEW (NCOL,NROW,NLAY)
3582      character FMT*20, ANAME*24
3583      C      -----
3584      C
3585      IFIRST=1                                AT 005F
3586      ICONST=1                               AT 0066
3587      C
3588      C1-----LOOP THROUGH ALL CELLS
3589      do J=1,NCOL                                AT 006D
3590.01      do I=1,NROW                                AT 008B
3591.01      C
3592.01      C2-----IF K > 0 THEN 2-D ARRAY, SET VALUES TO ZERO AT DRY/NO-FLOW CELLS
3593.01      C2----- (THIS AVOIDS THE LIKELIHOOD OF CELLS WITH UNREALISTIC VKD
3594.01      C2----- PARAMETERS BECOMING ACTIVE DUE TO REWETTING IN SUBSEQUENT
3595.01      C2----- SIMULATIONS) .
3596.02      if (K.gt.0) then                                AT 00A9
3597.03      if (IBOUND(J,I,K) .eq.0 .or. real (HNEW (J,I,K)) .eq.HDRY) then AT 00B5
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
3598.04      A(J,I)=0.0                                AT 00FD
3599.04      goto 10                                    AT 011D
3600.04      endif                                    AT 0122
3601.03      endif                                    AT 0122
3602.03      C
3603.03      C3-----CHECK IF ALL THE ACTIVE VALUES IN THE ARRAY ARE THE SAME.
3604.02      if (ICONST.eq.1) then                                AT 0122
3605.03      if (IFIRST.eq.1) then                                AT 012C
3606.04      ALAST=A(J,I)                                        AT 0136
3607.04      IFIRST=0                                          AT 015A
3608.04      else                                            AT 0161
3609.04      if (A(J,I) .ne. ALAST) then                            AT 0166
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
3610.05      ICONST=0                                          AT 0190
3611.05      ALAST=1.0                                         AT 0197
3612.05      endif                                            AT 01AB
3613.04      endif                                            AT 01AB
3614.03      endif                                            AT 01AB
3615.02      10      continue                                  AT 01AB
3616.02      enddo                                           AT 01AB
3617.01      enddo                                           AT 01B0
3618.01      C
3619.01      C4-----IF ALL ACTIVE VALUES ARE THE SAME WRITE A SINGLE VALUE.
3620      if (ICONST.eq.1) then                                AT 01B5
3621.01      write (IBCFOUT,56) 0,ALAST,FMT,ANAME,K           AT 01BF
3622.01      else                                            AT 0247
3623.01      C
3624.01      C5-----OTHERWISE WRITE OUT THE FULL ARRAY.
3625.01      write (IBCFOUT,56) INBCF,ALAST,FMT,ANAME,K       AT 024C
3626.01      do I=1,NROW                                       AT 02D2
3627.02      write (IBCFOUT,FMT) (A(J,I) ,J=1,NCOL)           AT 02F6
3628.02      enddo                                           AT 036B
3629.01      endif                                            AT 0370
3630.01      C
3631.01      C-----HEADER FORMAT (PRINTING TO 2ND OUTPUT FILE IS NOT REPRESSED) .
3632      56 format (i10,g10.3,a20,8x, ' 0',a24, ' Layer',i4)   AT 0370
3633      C
3634      C6-----RETURN
3635      return                                                AT 03B3
3636      end                                                    AT 03B8
3637      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<

```

End of compilation - Clocked 0.1 seconds

APPENDIX B
Modified computer code for stream package
with changes highlighted

COMPILER OPTIONS: listing intl no_persist nodclvar nomap nocheck logl dynm offset dreal noansi
nopagethrow

nosilent no_optimise warn73 nolink no_link

```

0001 C-Changes to the code are highlighted with the following headings:
0002 C
0003 C-Environment Agency (UK)-13.Allow an inflow to any stream reach>>>>>>>
0004 C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0005 C-Environment Agency (UK)-15.Save single flow if >1 stream in a cell>>>>
0006 C
0007 C These headings are followed by the original USGS MODFLOW-96 code
0008 C (commented out), followed by the modified code. All the code changes
0009 C are followed by the following:
0010 C
0011 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0012 C
0013 C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0014 C SUBROUTINE STR1AL(ISUM,LENX,LCSTRM,ICSTRM,MXSTRM,NSTREM,IN,
0015 C 1 IOUT,ISTCB1,ISTCB2,NSS,NTRIB,NDIV,ICALC,CONST,
0016 C 2 LCTBAR,LCTTRIB,LCIVAR,LCFGAR)
0017 SUBROUTINE STR1AL(ISUM,LENX,LCSTRM,ICSTRM,MXSTRM,NSTREM,IN,
0018 1 IOUT,ISTCB1,ISTCB2,NSS,NTRIB,NDIV,ICALC,CONST,
0019 2 LCTBAR,LCTTRIB,LCIVAR,LCFGAR, iswabs, lctba2)
0020 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0021 C C
0022 C-----VERSION 2 18DEC1990 STR1AL C
0023 C ***** C
0024 C ALLOCATE ARRAY STORAGE FOR STREAMS C
0025 C ***** C
0026 C C
0027 C SPECIFICATIONS: C
0028 C -----C
0029 C -----C
0030 C C
0031 C1-----IDENTIFY PACKAGE AND INITIALIZE NSTREM. C
0032 WRITE(IOUT,1) IN AT 0018
0033 C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0034 c 1 FORMAT(1H0,'STRM -- STREAM PACKAGE, VERSION 2, 12/18/90 ',
0035 c 1'INPUT READ FROM UNIT',I3)
0036 1 FORMAT(1H0,'STR-VKD1 -- STREAM PACKAGE, Allows inflows/outflows', AT 004E
0037 1' and tributary inflows at any stream cell, VERSION 1, 18/7/2001',
0038 1'INPUT READ FROM UNIT',I3)
0039 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0040 NSTREM=0 AT 00FD
0041 C C
0042 C2----- READ MXSTRM, NSS, NTRIB, ISTCB1, AND ISTCB2. C
0043 C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0044 c 100 READ(IN,3)MXSTRM,NSS,NTRIB,NDIV,ICALC,CONST,ISTCB1,ISTCB2
0045 c 3 FORMAT(5I10,F10.0,2I10)
0046 100 READ(IN,3)MXSTRM,NSS,NTRIB,NDIV,ICALC,CONST,ISTCB1,ISTCB2, iswabs AT 0106
0047 3 FORMAT(5I10,F10.0,3I10) AT 01BC
0048 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0049 IF(MXSTRM.LT.0)MXSTRM=0 AT 01DF
0050 IF(NSS.LT.0)NSS=0 AT 01F1
0051 WRITE(IOUT,4)MXSTRM,NSS,NTRIB AT 0203
0052 4 FORMAT(1H , 'MAXIMUM OF',I5, ' STREAM NODES'//1X, 'NUMBER OF STREAM S
0053 1EGMENTS IS ',I5//1X, 'NUMBER OF STREAM TRIBUTARIES IS ',I5//) AT 0259
0054 IF(NDIV.GT.0) WRITE(IOUT,5) AT 02FA
0055 5 FORMAT(1H , 'DIVERSIONS FROM STREAMS HAVE BEEN SPECIFIED') AT 032C
0056 IF(ICALC.GT.0) WRITE(IOUT,6) CONST AT 0371
0057 6 FORMAT(1H , 'STREAM STAGES WILL BE CALCULATED USING A CONSTANT OF
0058 1',F10.4) AT 03B3
0059 IF(ISTCB1.GT.0) WRITE(IOUT,7) ISTCB1,ISTCB2 AT 040A
0060 7 FORMAT(1X, 'CELL BUDGETS WILL BE SAVED ON UNITS',I3, 'AND',I3) AT 045C
0061 C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0062 if(iswabs.lt.0) write(iout,11) AT 04AB
0063 11 format(1X, 'SURFACE WATER ABSTRACTIONS AND DISCHARGES ALLOWED IN *A
0064 1NY* STREAM CELL') AT 04DD
0065 if(iswabs.gt.0) write(iout,12) AT 053A
0066 12 format(1X, 'SURFACE WATER ABSTRACTIONS, DISCHARGES AND TRIBUTARY IN
0067 1FLOWS ALLOWED IN *ANY* STREAM CELL') AT 056C
0068 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0069 C C
0070 C3-----SET LCSTRM EQUAL TO ADDRESS OF FIRST UNUSED SPACE IN X. C
0071 200 LCSTRM=ISUM AT 05DD
0072 C C
0073 C4-----CALCULATE AMOUNT OF SPACE NEEDED FOR STRM LIST. C
0074 ISPA=11*MXSTRM AT 05E7
0075 ISUM=ISUM+ISPA AT 05F7

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0076      C
0077      C5-----CALCULATE AMOUNT OF SPACE NEEDED FOR ISTRM LIST.
0078          ICSTRM=ISUM
0079          ISPB=5*MxSTRM
0080          ISUM=ISUM+ISPB
0081      C
0082      C6-----CALCULATE AMOUNT OF SPACE NEEDED FOR ITRBAR LIST.
0083          LCTBAR=ISUM
0084          ISPC=NSS*NTRIB
0085          ISUM=ISUM+ISPC
0086      C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0087          lctba2=isum
0088          if(iswabs.gt.0)isum=isum+ispc
0089      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0090      C
0091      C7-----CALCULATE AMOUNT OF SPACE NEEDED FOR ARTRIB LIST.
0092          LCTTRIB=ISUM
0093          ISPD=NSS
0094          ISUM=ISUM+ISPD
0095      C
0096      C8A-----CALCULATE AMOUNT OF SPACE NEEDED FOR IDIVAR LIST.
0097          LCTIVAR=ISUM
0098          ISPE=NSS
0099          ISUM=ISUM+ISPE
0100      C
0101      C8B-----CALCULATE AMOUNT IF SPACE NEEDED FOR NDFGAR LIST.
0102          LCFGAR=ISUM
0103          ISPF=NSS
0104          ISUM=ISUM+ISPF
0105          ISP=ISPA+ISPB+ISPC+ISPD+ISPE+ISPF
0106      C
0107      C9-----PRINT AMOUNT OF SPACE USED BY STREAM PACKAGE.
0108          WRITE (IOUT,8)ISP
0109          8 FORMAT(1X,I8,' ELEMENTS IN X ARRAY ARE USED FOR STREAMS')
0110          ISUM1=ISUM-1
0111          WRITE(IOUT,9) ISUM1,LENX
0112          9 FORMAT(1X,I8,' ELEMENTS OF X ARRAY USED OUT OF',I7)
0113          IF(ISUM1.GT.LENX) WRITE(IOUT,10)
0114          10 FORMAT(1X,' ***X ARRAY MUST BE DIMENSIONED LARGER***')
0115      C
0116      C10-----RETURN.
0117          RETURN
0118          END
0119      C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0120      c      SUBROUTINE STR1RP (STRM, ISTRM, NSTREM, MXSTRM, IN, IOUT, ITRBAR, NDIV,
0121      c      1      NSS, NTRIB, IDIVAR, ICALC, IPTFLG)
WARNING - Label 200 has not been referenced
WARNING - Label 100 has not been referenced

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0122          SUBROUTINE STR1RP (STRM, ISTRM, NSTREM, MXSTRM, IN, IOUT, ITRBAR, NDIV,
0123      1      NSS, NTRIB, IDIVAR, ICALC, IPTFLG, iswabs, itrba2)
0124      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0125      C
0126      C
0127      C-----VERSION 2 18DEC1990 STR1RP
0128      C *****
0129      C      READ STREAM DATA:  INCLUDES SEGMENT AND REACH NUMBERS, CELL
0130      C      SEQUENCE OF SEGMENT AND REACH, FLOW INTO MODEL AT BOUNDARY,
0131      C      STREAM STAGE, STREAMBED CONDUCTANCE, AND STREAMBED TOP AND
0132      C      BOTTOM ELEVATIONS
0133      C      *****
0134      C
0135      C      SPECIFICATIONS:
0136      C      -----C
0137      C      DIMENSION STRM(11, MXSTRM), ISTRM(5, MXSTRM), ITRBAR (NSS, NTRIB),
0138      1      IDIVAR (NSS)
0139      C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0140      dimension itrba2(nss,ntrib)
0141      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0142      C      -----C
0143      C
0144      C1A-----IF MXSTREAM IS LESS THAN 1 THEN STREAM IS INACTIVE. RETURN.
0145          IF (MXSTRM.LT.1) RETURN
0146      C
0147      C1B-----READ ITMP (NUMBER OF STREAM CELLS OR FLAG TO REUSE DATA) .
0148          READ (IN, 1) ITMP, IRDFLG, IPTFLG
0149          1 FORMAT(3I10)
0150      C
0151      C2A-----IF ITMP <0 THEN REUSE DATA FROM LAST STRESS PERIOD.
0152          IF (ITMP.GE.0) GO TO 50

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0153          WRITE(IOUT,2)
0154          2 FORMAT(1H0,'REUSING STREAM NODES FROM LAST STRESS PERIOD')
0155          RETURN
0156          C
0157          C2B-----IF ITMP=> ZERO THEN IT IS THE NUMBER OF STREAM REACHES.
0158          50 NSTREM=ITMP
0159          C
0160          C3A-----IF NSTREM>MXSTRM THEN STOP.
0161          IF(NSTREM.LE.MXSTRM)GO TO 100
0162          WRITE(IOUT,99)NSTREM,MXSTRM
0163          99 FORMAT(1H0,'NSTREM(',I4,') IS GREATER THAN MXSTRM(',I4,')')
0164          STOP
0165          C
0166          C3B-----PRINT NUMBER OF STREAM CELLS IN THIS STRESS PERIOD.
0167          100 IF(IRDFLG.EQ.0) WRITE(IOUT,3)NSTREM
0168          3 FORMAT(1H0,'//1X,I5,' STREAM NODES')
0169          C
0170          C4-----IF THERE ARE NO STREAM CELLS THEN RETURN.
0171          IF(NSTREM.EQ.0) RETURN
0172          C
0173          C5-----READ AND PRINT DATA FOR EACH STREAM CELL.
0174          IF(IRDFLG.EQ.0) WRITE(IOUT,4)
0175          4 FORMAT(1H,3X,'LAYER ROW COL SEGMENT REACH STREAMFLOW
0176          1 STREAM STREAMBED STREAMBED BOT STREAMBED TOP',/27X,
0177          2'NUMBER NUMBER STAGE CONDUCTANCE ELEVAT
0178          3ION ELEVATION',/3X,110('-'))
0179          DO 250 II=1,NSTREM
0180.01          READ(IN,5)K,I,J,ISTRM(4,II),ISTRM(5,II),STRM(1,II),STRM(2,II),
0181.01          1STRM(3,II),STRM(4,II),STRM(5,II)
0182.01          5 FORMAT(5I5,F15.0,4F10.0)
0183.01          IF(IRDFLG.EQ.0) WRITE(IOUT,6)K,I,J,ISTRM(4,II),ISTRM(5,II),
0184.01          1STRM(1,II),STRM(2,II),STRM(3,II),STRM(4,II),STRM(5,II)
0185.01          6 FORMAT(1X,3X,I4,2I7,2I9,7X,G11.4,G12.4,G11.4,4X,2G13.4)
0186.01          ISTRM(1,II)=K
0187.01          ISTRM(2,II)=I
0188.01          ISTRM(3,II)=J
0189.01          250 CONTINUE
0190.01          C
0191.01          C6----READ AND PRINT DATA IF STREAM STAGE IS CALCULATED.
0192          IF(ICALC.LE.0) GO TO 300
0193          IF(IRDFLG.EQ.0) WRITE(IOUT,7)
0194          7 FORMAT(1H0,3X,'LAYER',3X,'ROW',4X,'COL ', ' SEGMENT',3X,
0195          1'REACH',8X,'STREAM',13X,'STREAM',10X,'ROUGH',/27X,'NUMBER',3X,
0196          2 'NUMBER',8X,'WIDTH',14X,'SLOPE',10X,'COEF.',/3X,110('-'))
0197          DO 280 II=1,NSTREM
0198.01          READ(IN,8) STRM(6,II),STRM(7,II),STRM(8,II)
0199.01          8 FORMAT(3F10.0)
0200.01          IF(IRDFLG.EQ.0) WRITE(IOUT,9)ISTRM(1,II),ISTRM(2,II),ISTRM(3,II),
0201.01          1ISTRM(4,II),ISTRM(5,II),STRM(6,II),STRM(7,II),STRM(8,II)
0202.01          9 FORMAT(4X,I4,2I7,2I9,7X,G12.4,4X,G13.4,4X,G12.4)
0203.01          280 CONTINUE
0204.01          C
0205.01          C7-----INITIALIZE ALL TRIBUTARY SEGMENTS TO ZERO.
0206          300 DO 320 IK=1,NSS
0207.01          DO 320 JK=1,NTRIB
0208.02          ITRBAR(IK,JK)=0
0209.02          320 CONTINUE
0210.02          C
0211.02          C8-----INITIALIZE DIVERSION SEGMENT ARRAY TO ZERO.
0212          DO 325 IK=1,NSS
0213.01          IDIVAR(IK)=0
0214.01          325 CONTINUE
0215.01          C
0216.01          C9-----READ AND PRINT TRIBUTARY SEGMENTS.
0217          IF(NTRIB.LE.0) GO TO 343
0218          IF(IRDFLG.EQ.0) WRITE(IOUT,10)NTRIB
0219          C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0220          c 10 FORMAT(1H0,30X,'MAXIMUM NUMBER OF TRIBUTARY STREAMS IS ',I5,//1X,
0221          c 1 20X,'STREAM SEGMENT',15X,'TRIBUTARY STREAM SEGMENT NUMBERS')
0222          c DO 340 IK=1,NSS
0223          c READ(IN,11) (ITRBAR(IK,JK),JK=1,NTRIB)
0224          c 11 FORMAT(10I5)
0225          c IF(IRDFLG.EQ.0) WRITE(IOUT,12)IK,(ITRBAR(IK,JK),JK=1,NTRIB)
0226          c 12 FORMAT(20X,I5,20X,10I5)
0227          10 FORMAT(1H0,30X,'MAXIMUM NUMBER OF TRIBUTARY STREAMS IS ',I5,//1X,
0228          1 20X,'STREAM SEGMENT',15X,'TRIBUTARY SEGMENTS (INTO REACH)')
0229          DO 340 IK=1,NSS
0230.01          if(iswabs.gt.0)goto 331
0231.01          C
0232.01          C9A----USE ORIGINAL FORMAT
0233.01          READ(IN,11) (ITRBAR(IK,JK),JK=1,NTRIB)
0234.01          11 FORMAT(10I5)

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0314.01 C4----06FEB1990, CHECK FOR CELLS OUTSIDE MOVED TO C12, C16 AND C18. C
0315.01 C C
0316.01 C5-----DETERMINE STREAM SEGMENT AND REACH NUMBER. C
0317.01 ISTRG=ISTRM(4,L) AT 0176
0318.01 NREACH=ISTRM(5,L) AT 018D
0319.01 C C
0320.01 C-Environment Agency (UK)-13.Allow an inflow to any stream reach>>>>>>>
0321.01 cC6-----SET FLOWIN EQUAL TO STREAM SEGMENT INFLOW IF FIRST REACH. C
0322.01 c IF(NREACH.GT.1) GO TO 200
0323.01 c FLOWIN=STRM(1,L)
0324.01 C6-----SET FLOWIN EQUAL TO STREAM SEGMENT INFLOW IF any REACH. C
0325.01 C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0326.01 c FLOWIN=STRM(1,L)
0327.01 c IF(NREACH.GT.1) GO TO 200
0328.01 IF(iswabs.eq.0.and.NREACH.GT.1) GO TO 200 AT 01A4
0329.01 FLOWIN=STRM(1,L) AT 01B9
0330.01 IF(iswabs.lt.0.and.NREACH.GT.1) GO TO 200 AT 01DF
0331.01 IF(NREACH.GT.1) GO TO 60 AT 01F8
0332.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0333.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0334.01 C C
0335.01 C7-----STORE OUTFLOW FROM PREVIOUS SEGMENT IN ARTRIB IF SEGMENT >1. C
0336.01 IF(ISTRG.EQ.1)GO TO 50 AT 0205
0337.01 IFLG = ISTRM(4,LL) AT 0212
0338.01 ARTRIB(IFLG)=STRM(9,LL) AT 022C
0339.01 C C
0340.01 C8A-----CHECK UPSTREAM SEGMENT FOR DIVERSIONS. C
0341.01 DO 40 NSFLG = 1,NSS AT 0259
0342.02 IF(IFLG.NE.IDIVAR(NSFLG)) GO TO 40 AT 0286
0343.02 C C
0344.02 C8B-----DETERMINE AMOUNT OF FLOW TO BE DIVERTED. C
0345.02 DO 20 IDL=1,NSTREM AT 0299
0346.03 IF(NSFLG.NE.ISTRM(4,IDL)) GO TO 20 AT 02C6
0347.03 IF(ISTRM(5,IDL).NE.1) GO TO 20 AT 02E6
0348.03 DUM=ARTRIB(IFLG)-STRM(1,IDL) AT 0304
0349.03 C C
0350.03 C8C-----SUBTRACT FLOW FROM UPSTREAM SEGMENT IF THERE IS ENOUGH FLOW C
0351.03 C-----IN UPSTREAM SEGMENT. C
0352.03 IF(DUM.GE.0.0) ARTRIB(IFLG)=DUM AT 032E
0353.03 IF(DUM.LT.0.0) NDFGAR(IFLG)=1 AT 0358
0354.03 20 CONTINUE AT 037F
0355.02 40 CONTINUE AT 0384
0356.01 50 IF(IDIVAR(ISTRG).LE.0) GO TO 60 AT 0389
0357.01 NDFLG=IDIVAR(ISTRG) AT 039D
0358.01 IF(NDFGAR(NDFLG).EQ.1) FLOWIN=0.0 AT 03A7
0359.01 C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>>
0360.01 c 60 IF(FLOWIN.GE.0.0) GO TO 300
0361.01 60 IF(FLOWIN.GE.0.0.and.iswabs.eq.0) GO TO 300 AT 03C9
0362.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0363.01 C C
0364.01 C9-----SUM TRIBUTARY OUTFLOW AND USE AS INFLOW INTO DOWNSTREAM SEGMENT.C
0365.01 C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0366.01 c FLOWIN =0.
0367.01 if(iswabs.eq.0)FLOWIN =0. AT 03EB
0368.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0369.01 DO 100 ITRIB=1,NTRIB AT 040B
0370.02 INODE=ITRIBAR(ISTRG,ITRIB) AT 0438
0371.02 IF(INODE.LE.0) GO TO 100 AT 045A
0372.02 C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0373.02 if(iswabs.gt.0)then AT 0463
0374.03 if(itrba2(istsg,itrib).ne.nreach)goto 100 AT 046F
0375.03 endif AT 049D
0376.03 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0377.02 FLOWIN=FLOWIN+ARTRIB(INODE) AT 049D
0378.02 100 CONTINUE AT 04B7
0379.02 C C
0380.02 C-Environment Agency (UK)-13.Allow an inflow to any stream reach>>>>>>>
0381.02 cC10-----IF REACH >1, SET INFLOW EQUAL TO OUTFLOW FROM UPSTREAM REACH. C
0382.02 c 200 IF(NREACH.GT.1) FLOWIN=STRM(9,LL)
0383.02 C10-----IF REACH >1, add OUTFLOW FROM UPSTREAM REACH to inflow. C
0384.02 C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0385.02 c 200 IF(NREACH.GT.1) FLOWIN=flowin+STRM(9,LL)
0386.01 200 if(iswabs.eq.0)then AT 04BC
0387.02 IF(NREACH.GT.1) FLOWIN=STRM(9,LL) AT 04C8
0388.02 else AT 04FD
0389.02 IF(NREACH.GT.1) FLOWIN=flowin+STRM(9,LL) AT 0502
0390.02 endif AT 0534
0391.02 C C
0392.02 C10a---LIMIT SURFACE WATER ABSTRACTION IF NOT ENOUGH FLOW IN STREAM C
0393.01 if(iswabs.ne.0.and.flowin.lt.0)then AT 0534
0394.02 flowin=0.0 AT 0556
0395.02 endif AT 056A

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0396.02 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0397.02 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0398.02 C
0399.02 C11----COMPUTE STREAM STAGE IN REACH IF ICALC IS GREATER THAN 1. C
0400.01 300 IF (ICALC.LE.0) GO TO 310 AT 056A
0401.01 XNUM= ( (FLOWIN+STRM(9,L) ) /2.0) *STRM(8,L) AT 0576
0402.01 DNOM=CONST*STRM(6,L) * (SQRT (STRM(7,L) ) ) AT 05B4
0403.01 DEPTH= (XNUM/DNOM) **0.6 AT 05EA
0404.01 IF (DEPTH.LE.0.) DEPTH=0. AT 060F
0405.01 STRM(2,L) =DEPTH+STRM(5,L) AT 0633
0406.01 310 HSTR=STRM(2,L) AT 0665
0407.01 C C
0408.01 C12----DETERMINE LEAKAGE THROUGH STREAMBED. C
0409.01 IF (IBOUND(IC,IR,IL) .LE.0) GO TO 315 AT 068D
0410.01 IF (FLOWIN.LE.0.) HSTR=STRM(5,L) AT 06C1
0411.01 CSTR=STRM(3,L) AT 06FC
0412.01 SBOT=STRM(4,L) AT 0724
0413.01 H=HNEW(IC,IR,IL) AT 0749
0414.01 T=HSTR-SBOT AT 0780
0415.01 C C
0416.01 C13----COMPUTE LEAKAGE AS A FUNCTION OF STREAM STAGE AND HEAD IN CELL. C
0417.01 FLOBOT=CSTR* (HSTR-H) AT 0793
0418.01 C C
0419.01 C14----RECOMPUTE LEAKAGE IF HEAD IN CELL IS BELOW STREAMBED BOTTOM. C
0420.01 IQFLG=0 AT 07AC
0421.01 IF (H.GT.SBOT) GO TO 312 AT 07B6
0422.01 IQFLG=1 AT 07CC
0423.01 FLOBOT=CSTR*T AT 07D6
0424.01 C C
0425.01 C15----SET LEAKAGE EQUAL TO STREAM INFLOW IF LEAKAGE MORE THAN INFLOW. C
0426.01 312 IF (FLOBOT.LE.FLOWIN) GO TO 320 AT 07E9
0427.01 IQFLG=1 AT 07FF
0428.01 FLOBOT=FLOWIN AT 0809
0429.01 C C
0430.01 C16----STREAMFLOW OUT EQUALS STREAMFLOW IN MINUS LEAKAGE. C
0431.01 315 IF (IBOUND(IC,IR,IL) .LE.0) FLOBOT=0. AT 0821
0432.01 320 FLOWOT=FLOWIN-FLOBOT AT 0869
0433.01 IF ( (ISTSG.GT.1) .AND. (NREACH.EQ.1) ) STRM(9,LL) =ARTRIB (IFLG) AT 087C
0434.01 C C
0435.01 C17----STORE STREAM INFLOW, OUTFLOW AND LEAKAGE FOR EACH REACH. C
0436.01 STRM(9,L) =FLOWOT AT 08C3
0437.01 STRM(10,L) =FLOWIN AT 08EB
0438.01 STRM(11,L) =FLOBOT AT 0910
0439.01 C C
0440.01 C18----RETURN TO STEP 3 IF STREAM INFLOW IS LESS THAN OR EQUAL TO ZERO C
0441.01 C AND LEAKAGE IS GREATER THAN OR EQUAL TO ZERO OR IF CELL C
0442.01 C IS NOT ACTIVE--IBOUND IS LESS THAN OR EQUAL TO ZERO. C
0443.01 IF (IBOUND(IC,IR,IL) .LE.0) GO TO 500 AT 0935
0444.01 IF ( (FLOWIN.LE.0.0) .AND. (FLOBOT.GE.0.0) ) GO TO 500 AT 0969
0445.01 C C
0446.01 C19-----IF HEAD > BOTTOM THEN ADD TERMS TO RHS AND HCOF. C
0447.01 IF (IQFLG.GT.0) GO TO 400 AT 0995
0448.01 RHS (IC,IR,IL) =RHS (IC,IR,IL) -CSTR*HSTR AT 09A2
0449.01 HCOF (IC,IR,IL) =HCOF (IC,IR,IL) -CSTR AT 09DC
0450.01 GO TO 500 AT 0A0E
0451.01 C C
0452.01 C20-----IF HEAD < BOTTOM THEN ADD TERM ONLY TO RHS. C
0453.01 400 RHS (IC,IR,IL) =RHS (IC,IR,IL) -FLOBOT AT 0A13
0454.01 500 CONTINUE AT 0A45
0455.01 C C
0456.01 C21----RETURN. C
0457 RETURN AT 0A4A
0458 END AT 0A4F
0459 C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0460 c SUBROUTINE STR1BD (NSTREM,STRM,ISTRM,IBOUND,MXSTRM,HNEW,NCOL,NROW,
0461 c 1 NLAY,DELT,VBVL,VBNM,MSUM,KSTP,KPER,ISTCB1,ISTCB2,ICBCFL,BUFF,
0462 c 2 IOUT,NTRIB,NSS,ARTRIB,ITRBAR,IDIVAR,NDFGAR,ICALC,CONST,IPTFLG)

0463 SUBROUTINE STR1BD (NSTREM,STRM,ISTRM,IBOUND,MXSTRM,HNEW,NCOL,NROW,
0464 1 NLAY,DELT,VBVL,VBNM,MSUM,KSTP,KPER,ISTCB1,ISTCB2,ICBCFL,BUFF,
0465 2 IOUT,NTRIB,NSS,ARTRIB,ITRBAR,IDIVAR,NDFGAR,ICALC,CONST,IPTFLG,
0466 3 iswabs,itrba2)
0467 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0468 C-----VERSION 2 18DEC1990 STR1BD C
0469 C C
0470 C ***** C
0471 C CALCULATE VOLUMETRIC BUDGET FOR STREAMS C
0472 C ***** C
0473 C C
0474 C SPECIFICATIONS: C

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0475 C -----C
0476 CHARACTER*4 VBNM,TEXT,STRTXT
0477 DOUBLE PRECISION HNEW
0478 DIMENSION STRM(11,MXSTRM),ISTRM(5,MXSTRM),IBOUND(NCOL,NROW,NLAY),
0479 1 HNEW(NCOL,NROW,NLAY),VBVL(4,20),VBNM(4,20),
0480 2 BUFF(NCOL,NROW,NLAY),ARTRIB(NSS),ITRBAR(NSS,NTRIB),
0481 3 IDIVAR(NSS),NDFGAR(NSS)
0482 C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0483 dimension itrba2(nss,ntrib)
0484 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0485 DIMENSION TEXT(4),STRTXT(4)
0486 DATA TEXT(1),TEXT(2),TEXT(3),TEXT(4) /' ST','REAM',' LEA','KAGE'/ AT 00E0
0487 DATA STRTXT(1),STRTXT(2),STRTXT(3),STRTXT(4) /'STRE','AM F', AT 00E0
0488 1 'LOW ','OUT '/
0489 C -----C
0490 C C
0491 C1-----SET IBD=1 IF BUDGET TERMS SHOULD BE SAVED ON DISK. C
0492 IBD=0 AT 00E0
0493 RATIN = 0. AT 00EA
0494 RATOUT = 0. AT 00FE
0495 C C
0496 C2-----IF NO REACHES, KEEP ZEROS IN ACCUMULATORS. C
0497 IF(NSTREM.EQ.0) GO TO 600 AT 0112
0498 C C
0499 C3A-----TEST TO SEE IF CELL-BY-CELL TERMS ARE NEEDED. C
0500 IF((ICBCFL.EQ.0).OR.(ISTCB1.LE.0)) GO TO 10 AT 0121
0501 C C
0502 C3B-----CELL-BY-CELL TERMS ARE NEEDED, SET IBD AND CLEAR BUFFER. C
0503 IBD = 1 AT 0139
0504 DO 5 IL=1,NLAY AT 0143
0505.01 DO 5 IR=1,NROW AT 0170
0506.02 DO 5 IC=1,NCOL AT 019D
0507.03 BUFF(IC,IR,IL)=0. AT 01CA
0508.03 5 CONTINUE AT 01FF
0509.03 C C
0510.03 C3C-----INITIALIZE NDFGAR ARRAY TO ZERO. C
0511 DO 7 I=1,NSS AT 0208
0512.01 NDFGAR(I)=0 AT 0235
0513.01 7 CONTINUE AT 0240
0514.01 C C
0515.01 C4-----IF THERE ARE STREAMS THEN ACCUMULATE LEAKAGE TO OR FROM THEM. C
0516 10 DO 500 L=1,NSTREM AT 0242
0517.01 LL=L-1 AT 0272
0518.01 C C
0519.01 C5---DETERMINE REACH LOCATION. C
0520.01 IL=ISTRM(1,L) AT 0279
0521.01 IR=ISTRM(2,L) AT 0294
0522.01 IC=ISTRM(3,L) AT 02AB
0523.01 C C
0524.01 C6----06FEB1990, CHECK FOR CELLS OUTSIDE MOVED TO C14, C18 AND C29. C
0525.01 C C
0526.01 C7-----DETERMINE SEGMENT AND REACH NUMBER. C
0527.01 ISTSG=ISTRM(4,L) AT 02C2
0528.01 NREACH=ISTRM(5,L) AT 02D9
0529.01 C-Environment Agency (UK)-13.Allow an inflow to any stream reach>>>>>>>
0530.01 c IF(NREACH.GT.1) GO TO 200
0531.01 cC C
0532.01 cC8-----SET FLOWIN EQUAL TO SEGMENT INFLOW IF FIRST REACH. C
0533.01 c FLOWIN=STRM(1,L)
0534.01 C C
0535.01 C8-----SET FLOWIN EQUAL TO SEGMENT INFLOW IF any REACH. C
0536.01 C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0537.01 c FLOWIN=STRM(1,L)
0538.01 c IF(NREACH.GT.1) GO TO 200
0539.01 IF(iswabs.eq.0.and.NREACH.GT.1) GO TO 200 AT 02F0
0540.01 FLOWIN=STRM(1,L) AT 0305
0541.01 IF(iswabs.lt.0.and.NREACH.GT.1) GO TO 200 AT 032E
0542.01 IF(NREACH.GT.1) GO TO 60 AT 0347
0543.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0544.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0545.01 C C
0546.01 C9-----STORE OUTFLOW FROM PREVIOUS SEGMENT IN ARTRIB IF SEGMENT >1. C
0547.01 IF(ISTSG.EQ.1) GO TO 50 AT 0354
0548.01 IFLG = ISTRM(4,LL) AT 0361
0549.01 ARTRIB(IFLG)=STRM(9,LL) AT 037E
0550.01 C C
0551.01 C10A---CHECK UPSTREAM SEGMENT FOR DIVERSIONS. C
0552.01 DO 40 NSFLG = 1,NSS AT 03AE
0553.02 IF(IFLG.NE.IDIVAR(NSFLG)) GO TO 40 AT 03DB
0554.02 C C
0555.02 C10B---DETERMINE AMOUNT OF FLOW TO BE DIVERTED. C
0556.02 DO 20 IDL=1,NSTREM AT 03EE

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0557.03      IF(NSFLG.NE.ISTRM(4,IDL)) GO TO 20      AT 041E
0558.03      IF(ISTRM(5,IDL).NE.1) GO TO 20          AT 0441
0559.03      DUM=ARTRIB(IFLG)-STRM(1,IDL)           AT 045F
0560.03      C                                     C
0561.03      C10C---SUBTRACT FLOW FROM UPSTREAM SEGMENT IF THERE IS ENOUGH FLOW      C
0562.03      C      IN UPSTREAM SEGMENT.           C
0563.03      IF(DUM.GE.0.0) ARTRIB(IFLG)=DUM      AT 048C
0564.03      IF(DUM.LT.0.0) NDFGAR(IFLG)=1        AT 04B6
0565.03      20 CONTINUE                          AT 04DD
0566.02      40 CONTINUE                          AT 04E2
0567.01      50 IF(IDIVAR(ISTSG).LE.0) GO TO 60   AT 04E7
0568.01      NDFLG=IDIVAR(ISTSG)                 AT 04FB
0569.01      IF(NDFGAR(NDFLG).EQ.1) FLOWIN=0.0   AT 0505
0570.01      C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>>
0571.01      c 60 IF(FLOWIN.GE.0.0) GO TO 300
0572.01      60 IF(FLOWIN.GE.0.0.and.iswabs.eq.0) GO TO 300      AT 0527
0573.01      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0574.01      C                                     C
0575.01      C11--SUM TRIBUTARY OUTFLOW AND USE AS INFLOW INTO DOWNSTREAM SEGMENT. C
0576.01      C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>>
0577.01      c      FLOWIN =0.
0578.01      if(iswabs.eq.0)FLOWIN =0.           AT 0549
0579.01      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0580.01      DO 100 ITRIB=1,NTRIB                AT 0569
0581.02      INODE=ITRBAR(ISTSG,ITRIB)          AT 0596
0582.02      IF(INODE.LE.0) GO TO 100           AT 05B8
0583.02      C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>>
0584.02      if(iswabs.gt.0)then
0585.03      if(itrba2(istsg,itrib).ne.nreach)goto 100      AT 05C1
0586.03      endif                                AT 05CD
0587.03      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0588.02      FLOWIN=FLOWIN+ARTRIB(INODE)        AT 05FB
0589.02      100 CONTINUE                        AT 0615
0590.02      C                                     C
0591.02      C-Environment Agency (UK)-13.Allow an inflow to any stream reach>>>>>>>>
0592.02      cC12----IF REACH >1, SET INFLOW EQUAL TO OUTFLOW FROM UPSTREAM REACH. C
0593.02      c 200 IF(NREACH.GT.1) FLOWIN=STRM(9,LL)
0594.02      C12----IF REACH >1, add OUTFLOW FROM UPSTREAM REACH to inflow.           C
0595.02      C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>>
0596.02      c 200 IF(NREACH.GT.1) FLOWIN=flowin+STRM(9,LL)
0597.01      200 if(iswabs.eq.0)then           AT 061A
0598.02      IF(NREACH.GT.1) FLOWIN=STRM(9,LL) AT 0626
0599.02      else                             AT 065E
0600.02      IF(NREACH.GT.1) FLOWIN=flowin+STRM(9,LL) AT 0663
0601.02      endif                             AT 0698
0602.02      C                                     C
0603.02      C12a---LIMIT SURFACE WATER ABSTRACTION IF NOT ENOUGH FLOW IN STREAM      C
0604.01      if(iswabs.ne.0.and.flowin.lt.0)then AT 0698
0605.02      write(iout,11)istsg,nreach,-strm(1,1),-strm(1,1)+flowin AT 06BA
0606.02      11 format('**SURFACE WATER ABSTRACTION FROM SEGMENT',I5,', REACH', AT 0784
0607.02      1 I5,' REDUCED FROM',G12.4,' TO',G12.4,' **')
0608.02      flowin=0.0                        AT 0809
0609.02      endif                             AT 081D
0610.02      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0611.02      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0612.02      C                                     C
0613.02      C13----COMPUTE STREAM STAGE IN REACH IF ICALC > 1.                       C
0614.01      300 IF(ICALC.LE.0) GO TO 310      AT 081D
0615.01      XNUM=( (FLOWIN+STRM(9,L))/2.0)*STRM(8,L) AT 0829
0616.01      DNOM=CONST*STRM(6,L)*(SQRT(STRM(7,L))) AT 086A
0617.01      DEPTH=(XNUM/DNOM)**0.6            AT 08A0
0618.01      IF((DEPTH).LE.0) DEPTH=0.        AT 08C5
0619.01      STRM(2,L)=DEPTH+STRM(5,L)        AT 08E9
0620.01      310 HSTR=STRM(2,L)               AT 091E
0621.01      C                                     C
0622.01      C14----DETERMINE LEAKAGE THROUGH STREAMBED.                            C
0623.01      IF(IBOUND(IC,IR,IL).LE.0) GO TO 315 AT 0949
0624.01      IF(FLOWIN.LE.0.0) HSTR=STRM(5,L) AT 0986
0625.01      CSTR=STRM(3,L)                   AT 09C1
0626.01      SBOT=STRM(4,L)                   AT 09EC
0627.01      H=HNEW(IC,IR,IL)                 AT 0A11
0628.01      T=HSTR-SBOT                       AT 0A4E
0629.01      C                                     C
0630.01      C15----COMPUTE LEAKAGE AS A FUNCTION OF STREAM STAGE AND HEAD IN CELL. C
0631.01      FLOBOT=CSTR*(HSTR-H)             AT 0A61
0632.01      C                                     C
0633.01      C16---RECOMPUTE LEAKAGE IF HEAD IN CELL IS BELOW STREAMBED BOTTOM.      C
0634.01      IF(H.GT.SBOT) GO TO 312          AT 0A7A
0635.01      FLOBOT=CSTR*T                     AT 0A90
0636.01      C                                     C
0637.01      C17----SET LEAKAGE EQUAL TO STREAM INFLOW IF LEAKAGE MORE THAN INFLOW. C
0638.01      312 IF(FLOBOT.LE.FLOWIN) GO TO 320 AT 0AA3

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0639.01      FLOBOT=FLOWIN                                     AT 0AB9
0640.01      C
0641.01      C18----STREAMFLOW OUT EQUALS STREAMFLOW IN MINUS LEAKAGE.      C
0642.01      315 IF(IBOUND(IC,IR,IL).LE.0) FLOBOT=0.                                     AT 0AD1
0643.01      320 FLOWOT=FLOWIN-FLOBOT                                             AT 0B22
0644.01      IF((ISTSG.GT.1).AND.(NREACH.EQ.1)) STRM(9,LL)=ARTRIB(IFLG)          AT 0B35
0645.01      C
0646.01      C19----STORE STREAM INFLOW, OUTFLOW AND LEAKAGE FOR EACH REACH.      C
0647.01      STRM(9,L)=FLOWOT
0648.01      STRM(10,L)=FLOWIN
0649.01      STRM(11,L)=FLOBOT
0650.01      C
0651.01      C20----IF LEAKAGE FROM STREAMS IS TO BE SAVED THEN ADD RATE TO BUFFER. C
0652.01      IF(IBD.EQ.1) BUFF(IC,IR,IL)=BUFF(IC,IR,IL)+FLOBOT                    AT 0BF4
0653.01      C
0654.01      C21----DETERMINE IF FLOW IS INTO OR OUT OF MODEL CELL.              C
0655.01      C      SKIP ESTIMATE OF LEAKAGE FROM STREAM IF LEAKAGE IS ZERO.      C
0656.01      IF(FLOBOT)494,500,496                                               AT 0C39
0657.01      C
0658.01      C22-----SUBTRACT FLOW RATE FROM RATOUT IF AQUIFER DISCHARGES TO STREAM.C
0659.01      494 RATOUT=RATOUT-FLOBOT
0660.01      GO TO 500
0661.01      C
0662.01      C23-----ADD FLOW RATE TO RATIN IF STREAM DISCHARGES TO AQUIFER.      C
0663.01      496 RATIN=RATIN+FLOBOT
0664.01      500 CONTINUE
0665.01      C
0666.01      C24-----IF BUDGET TERMS WILL BE SAVED THEN WRITE TO DISK.          C
0667      IF(IBD.EQ.1) CALL UBUDSV(KSTP,KPER,TEXT,ISTCB1,BUFF,NCOL,NROW,
0668      1      NLAY,IOUT)
0669      C
0670      C25A-----MOVE RATES INTO VBVL FOR PRINTING BY MODULE BAS_OT.          C
0671      600 VBVL(3,MSUM)=RATIN
0672      VBVL(4,MSUM)=RATOUT
0673      C
0674      C25B-----MOVE PRODUCT OF RATE AND TIME STEP INTO VBVL ACCUMULATORS.      C
0675      VBVL(1,MSUM)=VBVL(1,MSUM)+RATIN*DELT
0676      VBVL(2,MSUM)=VBVL(2,MSUM)+RATOUT*DELT
0677      C
0678      C25C-----MOVE BUDGET TERM LABELS INTO VBNM FOR PRINTING BY BAS_OT.      C
0679      VBNM(1,MSUM)=TEXT(1)
0680      VBNM(2,MSUM)=TEXT(2)
0681      VBNM(3,MSUM)=TEXT(3)
0682      VBNM(4,MSUM)=TEXT(4)
0683      C
0684      C26-----INCREASE BUDGET TERM COUNTER BY ONE.                          C
0685      MSUM=MSUM+1
0686      C
0687      C27-----RESET IBD COUNTER TO ZERO.
0688      IBD=0
0689      C28-----IF STREAM OUTFLOW FROM EACH REACH IS TO BE STORED ON DISK      C
0690      THEN STORE OUTFLOW RATES TO BUFFER.
0691      IF((ICBCFL.EQ.0).OR.(ISTCB2.LE.0)) GO TO 625
0692      IBD = 1
0693      DO 605 IL=1,NLAY
0694.01      DO 605 IR=1,NROW
0695.02      DO 605 IC=1,NCOL
0696.03      605 BUFF(IC,IR,IL)=0.
0697.03      C
0698.03      C29-----SAVE STREAMFLOWS OUT OF EACH REACH ON DISK.                C
0699      DO 615 L=1,NSTREM
0700.01      IC=ISTRM(3,L)
0701.01      IR=ISTRM(2,L)
0702.01      IL=ISTRM(1,L)
0703.01      C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>>
0704.01      c      IF(IBOUND(IC,IR,IL).LE.0) GO TO 615
0705.01      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0706.01      C-Environment Agency (UK)-15.Save single flow if >1 stream in a cell>>>>
0707.01      c      BUFF(IC,IR,IL)=BUFF(IC,IR,IL)+STRM(9,L)
0708.01      BUFF(IC,IR,IL)=STRM(9,L)
0709.01      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0710.01      615 CONTINUE
0711      CALL UBUDSV(KSTP,KPER,STRTXT,ISTCB2,BUFF,NCOL,NROW,NLAY,IOUT)
0712      C
0713      C30-----PRINT STREAMFLOW RATES AND LEAKAGE FOR EACH REACH.              C
0714      625 IF((ISTCB1.GE.0).OR.(ICBCFL.LE.0)) GO TO 800
0715      IF(IPTFLG.GT.0) GO TO 800
0716      IF(ICALC.GT.0) GO TO 700
0717      WRITE(IOUT,650)
0718      650 FORMAT(1H0,12X,'LAYER',6X,'ROW',5X,'COLUMN',5X,'STREAM',4X,
0719      1'REACH',6X,'FLOW INTO',4X,'FLOW INTO',6X,'FLOW OUT OF'/43X,
0720      2      'NUMBER',3X,'NUMBER',4X,'STREAM REACH',4X,'AQUIFER',

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0721	3	6X, 'STREAM REACH'//)	
0722		DO 690 L=1,NSTREM	AT 10B1
0723.01		IL=ISTRM(1,L)	AT 10E1
0724.01		IR=ISTRM(2,L)	AT 10F6
0725.01		IC=ISTRM(3,L)	AT 110D
0726.01		WRITE(IOUT,675) IL, IR, IC, ISTRM(4,L), ISTRM(5,L),	AT 1124
0727.01	1	STRM(10,L), STRM(11,L), STRM(9,L)	
0728.01	675	FORMAT(1X,5X,5I10,8X,G9.3,5X,G9.3,8X,G9.3)	AT 1269
0729.01	690	CONTINUE	AT 12AA
0730		GO TO 800	AT 12AF
0731	700	WRITE(IOUT,710)	AT 12B4
0732	710	FORMAT(1H0,12X,'LAYER',6X,'ROW',5X,'COLUMN',5X,'STREAM',4X,	AT 12DA
0733		1'REACH',6X,'FLOW INTO',4X,'FLOW INTO',6X,'FLOW OUT OF',5X,	
0734		2'HEAD IN'/43X, 'NUMBER',3X,'NUMBER',4X,'STREAM REACH',	
0735		3 4X,'AQUIFER',6X,'STREAM REACH',5X,'STREAM'//)	
0736		DO 750 L=1,NSTREM	AT 13E5
0737.01		IL=ISTRM(1,L)	AT 1415
0738.01		IR=ISTRM(2,L)	AT 142A
0739.01		IC=ISTRM(3,L)	AT 1441
0740.01		WRITE(IOUT,775) IL, IR, IC, ISTRM(4,L), ISTRM(5,L),	AT 1458
0741.01	1	STRM(10,L), STRM(11,L), STRM(9,L), STRM(2,L)	
0742.01	775	FORMAT(1X,5X,5I10,8X,G9.3,5X,G9.3,7X,G9.3,4X,F9.2)	AT 15CC
0743.01	750	CONTINUE	AT 1619
0744	800	CONTINUE	AT 161E
0745	C		C
0746	C31----	RETURN.	C
0747		RETURN	AT 161E
0748		END	AT 1623

End of compilation - Clocked 0.0 seconds

APPENDIX C
Modified computer code for PCG solver package
with changes highlighted

COMPILER OPTIONS: listing intl no_persist nodclvar nomap nocheck logl dynm offset dreal noansi
 nopagethrow

nosilent no_optimise warn73 nolink no_link

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0001 C-Changes to the code are highlighted with the following headings:
0002 C
0003 C-Environment Agency (UK)-0.General change to enable new options>>>>>>>
0004 C-Environment Agency (UK)-10.Convergence info output to screen>>>>>>>>
0005 C-Environment Agency (UK)-11.Force converge if NOUTC outer itrns conv>>>>
0006 C-Environment Agency (UK)-12.Debugging output of unconverged heads>>>>>
0007 C
0008 C These headings are followed by the original USGS MODFLOW-96 code
0009 C (commented out), followed by the modified code. All the code changes
0010 C are followed by the following:
0011 C
0012 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0013 C-Environment Agency (UK)-12.Debugging output of unconverged heads>>>>>>>
0014 C- NOTE: The debugging option produces a file of all the
0015 C- heads calculated in the iteration process. This file is
0016 C- reset each time that a time step converges, so that only
0017 C- the information from an unconverged time step is kept. The
0018 C- outer iteration number is written to the part of the file
0019 C- that usually contains the stress period number, the inner
0020 C- iteration no. to the time step location, the largest head
0021 C- change to the stress period time location, and the largest
0022 C- flow residual to the total time location. The output file
0023 C- needs to be specified in the name file as DATA(BINARY), and
0024 C- the unit no. should be in columns 41-50 in the 1st line of
0025 C- the PCG input file.
0026 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0027 C
0028 C $Date: 1996/03/29 18:30:00 $
0029 C $Revision: 2.3 $
0030 C
0031 C-Environment Agency (UK)-0.General change to enable new options>>>>>>>
0032 c SUBROUTINE PCG2AL (ISUM, LENX, LCV, LCSS, LCP, LCCD, LCHCHG, LCLHCH,
0033 c 1 LCRCHG, LCLRCH, MXITER, ITER1, NCOL, NROW, NLAY, IN, IOUT, NPCOND,
0034 c A LCIT1)
0035 SUBROUTINE PCG2AL (ISUM, LENX, LCV, LCSS, LCP, LCCD, LCHCHG, LCLHCH,
0036 1 LCRCHG, LCLRCH, MXITER, ITER1, NCOL, NROW, NLAY, IN, IOUT, NPCOND,
0037 A LCIT1, noutc, ipcgdebug, iapart)
0038 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0039 C
0040 C-----VERSION 0002 01MAY1989 PCG2AL
0041 C
0042 C *****
0043 C ALLOCATE STORAGE IN THE X ARRAY FOR PCG ARRAYS
0044 C *****
0045 C
0046 C SPECIFICATIONS:
0047 C -----
0048 C -----
0049 C
0050 C-----PRINT A MESSAGE IDENTIFYING PCG PACKAGE
0051 WRITE(IOUT,1) AT 0018
0052 C-Environment Agency (UK)-0.General change to enable new options>>>>>>>
0053 c 1 FORMAT(1H0,'PCG2 -- CONJUGATE GRADIENT SOLUTION PACKAGE'
0054 c 1,', VERSION 2.1, 6/1/95')
0055 1 FORMAT(1H0,'PCG-VKD1 -- CONJUGATE GRADIENT SOLUTION PACKAGE' AT 003E
0056 1,', Including progress monitor & debugging option, 18/7/2001')
0057 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0058 C
0059 C-Environment Agency (UK)-0.General change to enable new options>>>>>>>
0060 C-----READ AND PRINT MXITER,ITER1 AND NPCOND
0061 c READ(IN,2) MXITER,ITER1,NPCOND
0062 c 2 FORMAT(3I10)
0063 c WRITE(IOUT,3) MXITER,ITER1,NPCOND
0064 c 3 FORMAT(' MAXIMUM OF',I4,' CALLS OF SOLUTION ROUTINE'/
0065 c 1 , ' MAXIMUM OF',I4,' INTERNAL ITERATIONS PER '
0066 c 2 , 'CALL TO SOLUTION ROUTINE'/
0067 c 3 , ' MATRIX PRECONDITIONING TYPE :',I5)
0068 READ(IN,2) MXITER,ITER1,NPCOND,noutc,ipcgdebug AT 00C5
0069 2 FORMAT(5I10) AT 013B
0070 WRITE(IOUT,3) MXITER,ITER1,NPCOND,noutc AT 0150
0071 3 FORMAT(' MAXIMUM OF',I4,' CALLS OF SOLUTION ROUTINE'/ AT 01B6
0072 1 , ' MAXIMUM OF',I4,' INTERNAL ITERATIONS PER '
0073 2 , 'CALL TO SOLUTION ROUTINE'/
0074 3 , ' MATRIX PRECONDITIONING TYPE :',I5/
0075 4 , ' CONVERGENCE WILL BE FORCED IF',I4,' CONSECUTIVE '
    
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0076          5          , 'OUTER ITERATIONS ARE WITHIN THE CONVERGENCE CRITERIA')
0077          if (ipcgdebug.gt.0) then
0078.01          if (iapart.ne.0) then
0079.02              write(iout,*)
0080.02              write(iout,*) '*** DEBUGGING OPTION ACTIVE ***'
0081.02              write(iout,*)
0082.02          else
0083.02              write(iout,*)
0084.02              write(iout,*) '*****'
0085.02              write(iout,*) '** DEBUGGING IS NOT ACTIVE BECAUSE IAPART=0 **'
0086.02              write(iout,*) '*****'
0087.02              write(iout,*)
0088.02              ipcgdebug=0
0089.02          endif
0090.01          endif
0091.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0092.01 C
0093.01 C-----ALLOCATE SPACE FOR THE PCG ARRAYS
0094          ISOLD=ISUM
0095          NRC=NROW*NCOL
0096          ISIZ=NRC*NLAY
0097          LCV=ISUM
0098          ISUM=ISUM+ISIZ
0099          LCSS=ISUM
0100          ISUM=ISUM+ISIZ
0101          LCP=ISUM
0102          ISUM=ISUM+ISIZ
0103          LCDD=ISUM
0104          IF (NPCOND.NE.2) ISUM=ISUM+ISIZ
0105          LCHCHG=ISUM
0106          ISUM=ISUM+MXITER*ITER1
0107          LCLHCH=ISUM
0108          ISUM=ISUM+3*MXITER*ITER1
0109          LCRCHG=ISUM
0110          ISUM=ISUM+MXITER*ITER1
0111          LCLRCH=ISUM
0112          ISUM=ISUM+3*MXITER*ITER1
0113          LCIT1=ISUM
0114          ISUM=ISUM+MXITER*ITER1
0115          C
0116          C-----CALCULATE AND PRINT THE SPACE USED IN THE X ARRAY
0117          ICG=ISUM-ISOLD
0118          WRITE(IOUT,4) ICG
0119          4 FORMAT(1X,I7,' ELEMENTS IN X ARRAY ARE USED BY PCG')
0120          ISUM1=ISUM-1
0121          WRITE(IOUT,5) ISUM1,LENX
0122          5 FORMAT(1X,I7,' ELEMENTS OF X ARRAY USED OUT OF',I7)
0123          IF (ISUM1.GT.LENX) WRITE(IOUT,6)
0124          6 FORMAT(1X,' ***X ARRAY MUST BE DIMENSIONED LARGER***')
0125          C
0126          C-----RETURN
0127          RETURN
0128          END

```

AT 02EF
 AT 02FB
 AT 0307
 AT 0321
 AT 0353
 AT 036D
 AT 0372
 AT 038C
 AT 03BE
 AT 03F0
 AT 0422
 AT 043C
 AT 0445
 AT 0445
 AT 0445
 AT 0445
 AT 045B
 AT 0464
 AT 046B
 AT 0470
 AT 047A
 AT 047F
 AT 0489
 AT 048E
 AT 0498
 AT 04A9
 AT 04B3
 AT 04C0
 AT 04C7
 AT 04D8
 AT 04DF
 AT 04EC
 AT 04F3
 AT 0504
 AT 050B
 AT 0518
 AT 0520
 AT 0557
 AT 0598
 AT 05A1
 AT 05E8
 AT 062B
 AT 065F
 AT 06A2
 AT 06A7

```

0129          SUBROUTINE PCG2RP (MXITER, ITER1, HCLOSE, RCLOSE, NPCOND, NBPOL,
0130          1          RELAX, IPRPCG, IN, IOUT, MUTPCG, NITER, IT1, DAMP)
0131          C
0132          C-----VERSION 0002 01MAY1989 PCG2RP
0133          C          01SEPT1990 IPCGCD OMITTED; NITER ADDED
0134          C          01JUNE1995 DAMP ADDED
0135          C
0136          C          *****
0137          C          READ DATA FOR PCG
0138          C          *****
0139          C
0140          C          SPECIFICATIONS:
0141          C          -----
0142          C          DIMENSION IT1 (MXITER*ITER1)
0143          C          -----
0144          C
0145          C-----READ HCLOSE, RCLOSE, RELAX, NBPOL, IPRPCG, MUTPCG
0146          READ (IN,1) HCLOSE, RCLOSE, RELAX, NBPOL, IPRPCG, MUTPCG, DAMP
0147          1 FORMAT(3F10.0,3I10,F10.0)
0148          C
0149          C-----PRINT MXITER, ITER1, NPCOND, HCLOSE, RCLOSE, RELAX, NBPOL, IPRPCG,
0150          C-----MUTPCG, DAMP
0151          WRITE(IOUT,100)
0152          100 FORMAT(1H0,///57X,'SOLUTION BY THE CONJUGATE-GRADIENT METHOD'
0153          1/57X,43('-'))
0154          WRITE(IOUT,115) MXITER

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AT 00E7
 AT 010D
 AT 0170

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0155      115 FORMAT(1H0,38X,'MAXIMUM NUMBER OF CALLS TO PCG ROUTINE =',I9)          AT 01A6
0156      WRITE(IOUT,120) ITER1                                                    AT 01F1
0157      120 FORMAT(1H ,42X,'MAXIMUM ITERATIONS PER CALL TO PCG =',I9)            AT 0227
0158      WRITE(IOUT,122) NPCOND                                                    AT 026E
0159      122 FORMAT(1H ,49X,'MATRIX PRECONDITIONING TYPE =',I9)                   AT 02A4
0160      IF (NPCOND.EQ.2) WRITE(IOUT,123)                                          AT 02E5
0161      123 FORMAT(1H ,58X,'THE MATRIX WILL BE SCALED')                           AT 0317
0162      WRITE(IOUT,124) RELAX,NBPOL                                                AT 034E
0163      124 FORMAT(1H ,26X,'RELAXATION FACTOR (ONLY USED WITH',                    AT 0394
0164      1' PRECOND. TYPE 1) =',E15.5,/,
0165      2 1H ,19X,'PARAMETER OF POLYOMIAL PRECOND.'
0166      3 , ' = 2 (2) OR IS CALCULATED :',I9)
0167      WRITE(IOUT,125) HCLOSE                                                    AT 044B
0168      125 FORMAT(1H ,43X,'HEAD CHANGE CRITERION FOR CLOSURE =',E15.5)           AT 0481
0169      WRITE(IOUT,127) RCLOSE                                                    AT 04CA
0170      127 FORMAT(1H ,39X,'RESIDUAL CHANGE CRITERION FOR CLOSURE =',E15.5)     AT 0500
0171      IF (IPRPGC.LE.0) IPRPCG=999                                              AT 054D
0172      WRITE(IOUT,130) IPRPCG,MUTPCG                                             AT 055F
0173      130 FORMAT(1H ,30X,'PCG HEAD AND RESIDUAL CHANGE PRINTOUT INTERVAL ='    AT 05A5
0174      1,I9,/,1H ,23X,'PRINTING FROM SOLVER IS LIMITED(1) OR ',
0175      2'SUPPRESSED (>1) =',I9)
0176      IF (DAMP.LE.0.0) DAMP=1.0                                                AT 064C
0177      WRITE(IOUT,135) DAMP                                                    AT 0671
0178      135 FORMAT(1H ,59X,'DAMPING PARAMETER =',E15.5)                         AT 06A7
0179      NITER=0                                                                    AT 06E0
0180      C
0181      RETURN                                                                    AT 06E9
0182      END                                                                        AT 06EE
0183      C-Environment Agency (UK)-0.General change to enable new options>>>>>>>
0184      C      SUBROUTINE PCG2AP (HNEW, IBOUND, CR, CC, CV, HCOF, RHS, V, SS, P, CD,
0185      C      1      HCHG, LHCH, RCHG, LRCH, KITER, NITER, HCLOSE, RCLOSE, ICNVG,
0186      C      2      KSTP, KPER, IPRPCG, MXITER, ITER1, NPCOND, NBPOL, NSTP, NCOL, NROW,
0187      C      3      NLAY, NODES, RELAX, IOUT, MUTPCG, IU, IP, SN, SP, SR, IT1, DAMP)

0188      SUBROUTINE PCG2AP (HNEW, IBOUND, CR, CC, CV, HCOF, RHS, V, SS, P, CD,
0189      1      HCHG, LHCH, RCHG, LRCH, KITER, NITER, HCLOSE, RCLOSE, ICNVG,
0190      2      KSTP, KPER, IPRPCG, MXITER, ITER1, NPCOND, NBPOL, NSTP, NCOL, NROW,
0191      3      NLAY, NODES, RELAX, IOUT, MUTPCG, IU, IP, SN, SP, SR, IT1, DAMP, noutc,
0192      4      nout, ipcgdebug, ixsec, chedfm, buff, lbhdsv)
0193      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0194      C-----VERSION 0002 01MAY1989 PCG2AP
0195      C      01JULY1990 COMMENT STATEMENTS ADDED AND MODIFIED
0196      C      01SEPT1990 IPCGCD OMITTED; STATEMENT 590 ADDED
0197      C      27SEPT1990 STATEMENT IN DO 155 LOOP CHANGED
0198      C      01SEPT1991 ADDED STATEMENTS RELATED TO SENSITIVITY CALCULATIONS
0199      C      AT THE END OF THE 115 LOOP. CHANGED THE 510 FORMAT
0200      C      STATEMENT AND THE PRECEDING IF STATEMENT
0201      C      20MAR1992 CHANGED 510 FORMAT STATEMENT; OMITTED 2 LINES IN DO 160
0202      C      LOOP
0203      C      01MAY1993 ADDED DEL TO CALCULATION OF THE CHOLESKY DIAGONAL
0204      C      15JUNE1993 MADE CELLS SURROUNDED BY DRY CELLS INACTIVE
0205      C      01JUNE1995 ADDED DAMP
0206      C
0207      C      *****
0208      C      SOLUTION BY THE CONJUGATE GRADIENT METHOD -
0209      C      UP TO ITER1 ITERATIONS
0210      C      *****
0211      C
0212      C      SPECIFICATIONS:
0213      C      -----
0214      C      PARAMETER (DZERO=0.D0,DONE=1.D0)
0215      C      DOUBLE PRECISION HNEW,HHCOF,RRHS,DEL
0216      C      DOUBLE PRECISION Z,B,D,E,F,H,S,ALPHA
0217      C      DOUBLE PRECISION ZHNEW,BHNEW,DHNEW,FHNEW,HHNEW,SHNEW
0218      C      DOUBLE PRECISION SRNEW,SROLD,SSCR,SSCC,SSCV,VCC,VCR,VCV
0219      C      DOUBLE PRECISION CDCC,CDCR,CDCV
0220      C      DOUBLE PRECISION PN,VN,HCHGN,RCHGN,PAP
0221      C      DOUBLE PRECISION FCC,FCR,FCV,FV
0222      C
0223      C      DIMENSION HNEW(NODES), IBOUND(NODES), CR(NODES), CC(NODES),
0224      C      1 CV(NODES), HCOF(NODES), RHS(NODES), IT1(MXITER*ITER1),
0225      C      2 V(NODES), SS(NODES), P(NODES), CD(NODES), HCHG(MXITER*ITER1),
0226      C      3 LHCH(3,MXITER*ITER1), RCHG(MXITER*ITER1), LRCH(3,MXITER*ITER1)
0227      C-Environment Agency (UK)-12.Debugging output of unconverged heads>>>>>
0228      C      dimension buff(nodes)
0229      C      character text*16,chedfm*20,fname*100,acc*10
0230      C      text='Unconverged Head'                                             AT 0059
0231      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0232      C      -----
0233      C

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0234      C      IF(NITER.EQ.0) THEN
0235      C      WRITE(IOUT,895)
0236      C      WRITE(IOUT,900) (I,CC(I),CR(I),CV(I),HCOF(I),
0237      C      1      RHS(I),HNEW(I),IBOUND(I),I=1,50)
0238      C      ENDIF
0239      895 FORMAT('      I',5X,'CC',10X,'CR',10X,'CV',9X,'HCOF',8X,'RHS',9X,
0240      1      'HNEW',4X,'IBOUND (IBND=0 NOT PRINTED)')
0241      900 FORMAT(I5,5E12.3,D12.3,I5)
0242      C-Environment Agency (UK)-12.Debugging output of unconverged heads>>>>>>
0243      if(ipcgdebug.gt.0.and.kiter.eq.1)then
0244.01      inquire(ipcgdebug,access=acc,name=fname)
0245.01      if(acc.eq.'DIRECT')then
0246.02      inquire(ipcgdebug,recl=irecl)
0247.02      close(ipcgdebug,status='delete')
0248.02      irecl=((ncol*nrow)+1)*4
0249.02      open(ipcgdebug,file=fname,access='direct',recl=irecl)
0250.02      else
0251.02      close(ipcgdebug,status='delete')
0252.02      open(ipcgdebug,file=fname,access='sequential')
0253.02      endif
0254.01      endif
0255.01      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0256.01      C-----ASSIGN VARIABLE EQUAL TO THE NUMBER OF CELLS IN ONE LAYER
0257      NRC=NROW*NCOL
0258      C-----INITIALIZE VARIABLES USED TO CALCULATE ITERATION PARAMETERS
0259      SRNEW=DZERO
0260      BPOLY=0.
0261      IF(NPCOND.NE.1) RELAX=1.
0262      NORM=0
0263      IF(NPCOND.EQ.2) NORM=1
0264      C-----INITIALIZE VARIABLE USED TO TEST FOR NEGATIVE CHOLESKY DIAGONAL
0265      CD1=0.
0266      C-----CLEAR PCG WORK ARRAYS.
0267      DO 100 N=1,NODES
0268.01      SS(N)=0.
0269.01      P(N)=0.
0270.01      100 V(N)=0.
0271.01      C-----FOR NPCOND=1, INITIALIZE CHOLESKY DIAGONAL
0272      IF(NPCOND.EQ.1) THEN
0273.01      DO 105 N=1,NODES
0274.02      105 CD(N)=0.
0275.01      ENDF
0276.01      C
0277.01      C-----CALCULATE THE RESIDUAL. IF NORM=1, CALCULATE THE DIAGONALS OF
0278.01      C-----THE A MATRIX,AND STORE THEM IN HCOF.
0279      DO 115 K=1,NLAY
0280.01      DO 115 I=1,NROW
0281.02      DO 115 J=1,NCOL
0282.02      C
0283.02      C-----CALCULATE 1 DIMENSIONAL SUBSCRIPT OF CURRENT CELL AND
0284.02      C-----SKIP CALCULATIONS IF CELL IS INACTIVE
0285.03      N=J+(I-1)*NCOL+(K-1)*NRC
0286.03      IF(IBOUND(N).EQ.0) THEN
0287.04      CC(N)=0.
0288.04      CR(N)=0.
0289.04      IF(N.LE.(NODES-NRC)) CV(N)=0.
0290.04      IF(N.GE.2) CR(N-1)=0.
0291.04      IF(N.GE.NCOL+1) CC(N-NCOL)=0.
0292.04      IF(N.LE.(NODES-NRC).AND.N.GE.NRC+1) CV(N-NRC)=0.
0293.04      HCOF(N)=0.
0294.04      RHS(N)=0.
0295.04      GO TO 115
0296.04      ENDF
0297.04      C
0298.04      C-----CALCULATE 1 DIMENSIONAL SUBSCRIPTS FOR LOCATING THE 6
0299.04      C-----SURROUNDING CELLS
0300.03      NRN=N+NCOL
0301.03      NRL=N-NCOL
0302.03      NCN=N+1
0303.03      NCL=N-1
0304.03      NLN=N+NRC
0305.03      NLL=N-NRC
0306.03      C
0307.03      C-----CALCULATE 1 DIMENSIONAL SUBSCRIPTS FOR CONDUCTANCE TO THE 6
0308.03      C-----SURROUNDING CELLS.
0309.03      NCF=N
0310.03      NCD=N-1
0311.03      NRB=N-NCOL
0312.03      NRH=N
0313.03      NLS=N
0314.03      NLZ=N-NRC
0315.03      C

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0316.03 C-----GET CONDUCTANCES TO NEIGHBORING CELLS
0317.03 C-----NEIGHBOR IS 1 ROW BACK
0318.03 B=DZERO AT 0665
0319.03 BHNEW=DZERO AT 0679
0320.03 IF (I.NE.1) THEN AT 068D
0321.04 B=CC (NRB) AT 069A
0322.04 BHNEW=B* (HNEW (NRL) -HNEW (N) ) AT 06BA
0323.04 ENDIF AT 06E1
0324.04 C
0325.04 C-----NEIGHBOR IS 1 ROW AHEAD
0326.03 H=DZERO AT 06E1
0327.03 HHNEW=DZERO AT 06F5
0328.03 IF (I.NE.NROW) THEN AT 0709
0329.04 H=CC (NRH) AT 071A
0330.04 HHNEW=H* (HNEW (NRN) -HNEW (N) ) AT 073A
0331.04 ENDIF AT 0761
0332.04 C
0333.04 C-----NEIGHBOR IS 1 COLUMN BACK
0334.03 D=DZERO AT 0761
0335.03 DHNEW=DZERO AT 0775
0336.03 IF (J.NE.1) THEN AT 0789
0337.04 D=CR (NCD) AT 0796
0338.04 DHNEW=D* (HNEW (NCL) -HNEW (N) ) AT 07B6
0339.04 ENDIF AT 07DD
0340.04 C
0341.04 C-----NEIGHBOR IS 1 COLUMN AHEAD
0342.03 F=DZERO AT 07DD
0343.03 FHNEW=DZERO AT 07F1
0344.03 IF (J.NE.NCOL) THEN AT 0805
0345.04 F=CR (NCF) AT 0816
0346.04 FHNEW=F* (HNEW (NCN) -HNEW (N) ) AT 0836
0347.04 ENDIF AT 085D
0348.04 C
0349.04 C-----NEIGHBOR IS 1 LAYER BEHIND
0350.03 Z=DZERO AT 085D
0351.03 ZHNEW=DZERO AT 0871
0352.03 IF (K.NE.1) THEN AT 0885
0353.04 Z=CV (NLZ) AT 0892
0354.04 ZHNEW=Z* (HNEW (NLL) -HNEW (N) ) AT 08B2
0355.04 ENDIF AT 08D9
0356.04 C
0357.04 C-----NEIGHBOR IS 1 LAYER AHEAD
0358.03 S=DZERO AT 08D9
0359.03 SHNEW=DZERO AT 08ED
0360.03 IF (K.NE.NLAY) THEN AT 0901
0361.04 S=CV (NLS) AT 0912
0362.04 SHNEW=S* (HNEW (NLN) -HNEW (N) ) AT 0932
0363.04 ENDIF AT 0959
0364.04 C
0365.03 IF (I.EQ.NROW) CC (N)=0. AT 0959
0366.03 IF (J.EQ.NCOL) CR (N)=0. AT 0986
0367.03 C-----15JUN1993 SKIP CALCULATIONS AND MAKE CELL INACTIVE IF ALL
0368.03 C SURROUNDING CELLS ARE INACTIVE
0369.03 IF (B+H+D+F+Z+S.EQ.0.) THEN AT 09B3
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
0370.04 IBOUND (N)=0 AT 09E7
0371.04 HCOF (N)=0. AT 09FB
0372.04 RHS (N)=0. AT 0A11
0373.04 GO TO 115 AT 0A27
0374.04 ENDIF AT 0A2C
0375.04 C
0376.04 C-----CALCULATE THE RESIDUAL AND STORE IT IN RHS. TO SCALE A,
0377.04 C-----CALCULATE THE DIAGONAL OF THE A MATRIX, AND STORE IT IN HCOF.
0378.03 E=-Z-B-D-F-H-S AT 0A2C
0379.03 RRHS=RHS (N) AT 0A59
0380.03 HHCOF=HNEW (N) *HCOF (N) AT 0A79
0381.03 RHS (N) =RRHS -ZHNEW -BHNEW -DHNEW -HHCOF -FHNEW -HHNEW -SHNEW AT 0A94
0382.03 IF (NORM.EQ.1) HCOF (N) =HCOF (N) +E AT 0AC5
0383.03 IF (IBOUND (N) .LT.0) RHS (N) =0. AT 0AE1
0384.03 C-----ADDED FOR SENSITIVITY CALCULATIONS 9/1/91
0385.03 IF (IU.NE.0.AND.IP.GT.0) THEN AT 0B0E
0386.04 IF (I.EQ.1.AND.J.EQ.1.AND.K.EQ.1) THEN AT 0B26
0387.05 SN=0. AT 0B4D
0388.05 SP=0. AT 0B5D
0389.05 SR=0. AT 0B6D
0390.05 ENDIF AT 0B7D
0391.04 SR=SR+RHS (N) AT 0B7D
0392.04 IF (RRHS.LT.0.) SN=SN+RRHS AT 0B95
0393.04 IF (RRHS.GT.0.) SP=SP+RRHS AT 0BB9
0394.04 IF (-ZHNEW.LT.0.) SN=SN-ZHNEW AT 0BDD
0395.04 IF (-ZHNEW.GT.0.) SP=SP-ZHNEW AT 0C03
0396.04 IF (-BHNEW.LT.0.) SN=SN-BHNEW AT 0C29

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0397.04      IF (-BHNEW.GT.0.) SP=SP-BHNEW      AT 0C4F
0398.04      IF (-DHNEW.LT.0.) SN=SN-DHNEW      AT 0C75
0399.04      IF (-DHNEW.GT.0.) SP=SP-DHNEW      AT 0C9B
0400.04      IF (-HHCOF.LT.0.) SN=SN-HHCOF      AT 0CC1
0401.04      IF (-HHCOF.GT.0.) SP=SP-HHCOF      AT 0CE7
0402.04      IF (-FHNEW.LT.0.) SN=SN-FHNEW      AT 0D0D
0403.04      IF (-FHNEW.GT.0.) SP=SP-FHNEW      AT 0D33
0404.04      IF (-HHNEW.LT.0.) SN=SN-HHNEW      AT 0D59
0405.04      IF (-HHNEW.GT.0.) SP=SP-HHNEW      AT 0D7F
0406.04      IF (-SHNEW.LT.0.) SN=SN-SHNEW      AT 0DA5
0407.04      IF (-SHNEW.GT.0.) SP=SP-SHNEW      AT 0DCB
0408.04      ENDIF
0409.03      115 CONTINUE      AT 0DF1
0410.03      C
0411.03      C-----SCALE CC,CR,CV,RHS AND HNEW IF NORM=1.
0412          IF (NORM.EQ.1) THEN      AT 0E00
0413.01          DO 120 K=1,NLAY      AT 0E0D
0414.02          DO 120 I=1,NROW      AT 0E3A
0415.03          DO 120 J=1,NCOL      AT 0E67
0416.04          N=J+(I-1)*NCOL+(K-1)*NRC      AT 0E94
0417.04          IF (IBOUND(N).EQ.0) GO TO 120      AT 0EB9
0418.04          HHCOF=SQRT (-HCOF(N))      AT 0ECA
0419.04          IF (N.LE.(NODES-NCOL).AND.CC(N).GT.0.)      AT 0EDF
0420.04          #      CC(N)=CC(N)/(HHCOF*(SQRT(-HCOF(N+NCOL))))
0421.04          IF (CR(N).GT.0.) CR(N)=CR(N)/(HHCOF*(SQRT(-HCOF(N+1))))      AT 0F2F
0422.04          IF (N.LE.(NODES-NRC).AND.CV(N).GT.0.)      AT 0F74
0423.04          #      CV(N)=CV(N)/(HHCOF*(SQRT(-HCOF(N+NRC))))
0424.04          HNEW(N)=HNEW(N)*HHCOF      AT 0FDC
0425.04          RHS(N)=RHS(N)/HHCOF      AT 0FF7
0426.04      120 CONTINUE      AT 100C
0427.01      ENDIF      AT 101B
0428.01      C
0429.01      C-----CALCULATE PARAMETER B OF THE POLYNOMIAL PRECONDITIONING METHOD
0430          IF (NPCOND.NE.2) GO TO 152      AT 101B
0431          IF (NBPOL.EQ.2) THEN      AT 1027
0432.01          BPOLY=2      AT 1033
0433.01          GO TO 151      AT 1047
0434.01          ENDIF      AT 104C
0435          DO 150 K=1,NLAY      AT 104C
0436.01          DO 150 I=1,NROW      AT 1079
0437.02          DO 150 J=1,NCOL      AT 10A6
0438.02      C
0439.03          N=J+(I-1)*NCOL+(K-1)*NRC      AT 10D3
0440.03          IF (IBOUND(N).LE.0) GO TO 150      AT 10F8
0441.03      C
0442.03          NCF=N      AT 1109
0443.03          NCD=N-1      AT 110F
0444.03          NRB=N-NCOL      AT 1116
0445.03          NRH=N      AT 1124
0446.03          NLS=N      AT 1130
0447.03          NLZ=N-NRC      AT 1136
0448.03      C
0449.03          B=DZERO      AT 1142
0450.03          IF (I.NE.1) B=CC(NRB)      AT 1156
0451.03          H=DZERO      AT 117D
0452.03          IF (I.NE.NROW) H=CC(NRH)      AT 1191
0453.03          D=DZERO      AT 11C2
0454.03          IF (J.NE.1) D=CR(NCD)      AT 11D6
0455.03          F=DZERO      AT 1203
0456.03          IF (J.NE.NCOL) F=CR(NCF)      AT 1217
0457.03          Z=DZERO      AT 1248
0458.03          IF (K.NE.1) Z=CV(NLZ)      AT 125C
0459.03          S=DZERO      AT 1289
0460.03          IF (K.NE.NLAY) S=CV(NLS)      AT 129D
0461.03      C
0462.03      C-----NOTE : ABS. VAL. OF THE DIAG. OF THE SCALED A MATRIX IS 1.
0463.03          HHCOF=HCOF(N)      AT 12CE
0464.03          IF (NORM.EQ.1) HHCOF=DONE      AT 12EE
0465.03          T=DABS(Z)+DABS(B)+DABS(D)+ABS(HHCOF)+DABS(F)+DABS(H)+DABS(S)      AT 130F
0466.03          IF (T.GT.BPOLY) BPOLY=T      AT 135A
0467.03      150 CONTINUE      AT 1382
0468          151 CONTINUE      AT 1391
0469      C
0470      C-----CALCULATE ITERATION PARAMETERS FOR POLYNOMIAL PRECONDITIONING
0471      C-----METHOD FOR A NEGATIVE DEFINITE MATRIX.
0472          C0=(15./32.)*(BPOLY**3)      AT 1391
0473          C1=(27./16.)*(BPOLY**2)      AT 13B0
0474          C2=(9./4.)*BPOLY      AT 13C9
0475          152 CONTINUE      AT 13DC
0476      C
0477      C-----START INTERNAL ITERATIONS
0478          IITER=0      AT 13DC

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0479          IF(KITER.EQ.1) NITER=0                                AT 13E6
0480          ICNVG=0                                              AT 1401
0481          IICNVG=0                                            AT 140D
0482    153    CONTINUE                                           AT 1417
0483          IITER=IITER+1                                        AT 1417
0484          NITER=NITER+1                                        AT 141D
0485    C
0486    C-----INITIALIZE VARIABLES THAT TRACK MAXIMUM HEAD CHANGE AND RESIDUAL
0487    C-----VALUE DURING EACH ITERATIONS
0488          BIGH=0.                                             AT 1425
0489          BIGR=0.                                             AT 1439
0490    C-----INITIALIZE DEL (ADDED 01MAY1993)
0491          DEL=0.                                             AT 144D
0492    C
0493    C
0494    C-----CHECK NPCOND FOR PRECONDITIONING TYPE AND EXECUTE PROPER CODE
0495          IF(NPCOND.EQ.2) GO TO 165                            AT 1461
0496    C
0497    C-----CHOLESKY PRECONDITIONING
0498    C
0499    C-----STEP THROUGH CELLS TO CALCULATE THE DIAGONAL OF THE CHOLESKY
0500    C-----MATRIX (FIRST INTERNAL ITERATION ONLY) AND THE INTERMEDIATE
0501    C-----SOLUTION. STORE THEM IN CD AND V, RESPECTIVELY.
0502    154    DO 155 K=1,NLAY                                     AT 146D
0503.01      DO 155 I=1,NROW                                     AT 149A
0504.02      DO 155 J=1,NCOL                                     AT 14C7
0505.02    C
0506.03      N=J+(I-1)*NCOL+(K-1)*NRC                          AT 14F4
0507.03      IF(IBOUND(N).LE.0)GO TO 155                       AT 1519
0508.03    C
0509.03    C-----CALCULATE V
0510.03      H=DZERO                                             AT 152A
0511.03      VCC=DZERO                                           AT 153E
0512.03      IC=N-NCOL                                           AT 1552
0513.03      IF(I.NE.1) THEN                                     AT 155A
0514.04        H=CC(IC)                                          AT 1567
0515.04        IF(CD(IC).NE.0.) VCC=H*V(IC)/CD(IC)             AT 1581
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
0516.04      ENDIF                                             AT 15BC
0517.04    C
0518.03      F=DZERO                                             AT 15BC
0519.03      VCR=DZERO                                           AT 15D0
0520.03      IR=N-1                                              AT 15E4
0521.03      IF(J.NE.1) THEN                                     AT 15F1
0522.04        F=CR(IR)                                          AT 15FE
0523.04        IF(CD(IR).NE.0.) VCR=F*V(IR)/CD(IR)             AT 1618
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
0524.04      ENDIF                                             AT 1653
0525.04    C
0526.03      S=DZERO                                             AT 1653
0527.03      VCV=DZERO                                           AT 1667
0528.03      IL=N-NRC                                           AT 167B
0529.03      IF(K.NE.1) THEN                                     AT 168D
0530.04        S=CV(IL)                                          AT 169A
0531.04        IF(CD(IL).NE.0.) VCV=S*V(IL)/CD(IL)             AT 16B4
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
0532.04      ENDIF                                             AT 16EF
0533.03      V(N)=RHS(N)-VCR-VCC-VCV                             AT 16EF
0534.03    C
0535.03    C-----CALCULATE CD - FIRST INTERNAL ITERATION ONLY
0536.03      IF(IITER.EQ.1) THEN                                  AT 171C
0537.04        CDCR=DZERO                                         AT 1729
0538.04        CDCC=DZERO                                         AT 173D
0539.04        CDCV=DZERO                                         AT 1751
0540.04        FCC=DZERO                                         AT 1765
0541.04        FCR=DZERO                                         AT 1779
0542.04        FCV=DZERO                                         AT 178D
0543.04        IF(IR.GT.0.AND.CD(IR).NE.0.) CDCR=(F**2)/CD(IR)  AT 17A1
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
0544.04        IF(IC.GT.0.AND.CD(IC).NE.0.) CDCC=(H**2)/CD(IC)  AT 17E1
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
0545.04        IF(IL.GT.0.AND.CD(IL).NE.0.) CDCV=(S**2)/CD(IL) AT 182B
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
0546.04      IF(NPCOND.EQ.1) THEN                                AT 1875
0547.05        IF(IR.GT.0) THEN                                    AT 1881
0548.06          FV=CV(IR)                                        AT 188E
0549.06    C          MODIFIED FROM HILL(1990) 9/27/90: 2 REPLACES 1
0550.06          IF(K.EQ.NLAY.AND.((J+I).GT.2)) FV=DZERO        AT 18AE
0551.06          IF(CD(IR).NE.0.) FCR=(F/CD(IR))*(CC(IR)+FV)    AT 18E8
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
0552.06      ENDIF                                             AT 1931
0553.05      IF(IC.GT.0) THEN                                    AT 1931

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0554.06          FV=CV(IC)                                AT 193E
0555.06          IF(K.EQ.NLAY.AND.(I.GT.1)) FV=DZERO     AT 195E
0556.06          IF(CD(IC).NE.0.) FCC=(H/CD(IC))*(CR(IC)+FV) AT 1990
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
0557.06          ENDIF                                    AT 19D9
0558.05          IF(IL.GT.0) THEN                          AT 19D9
0559.06          IF(CD(IL).NE.0.) FCV=(S/CD(IL))*(CR(IL)+CC(IL)) AT 19E6
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
0560.06          ENDIF                                    AT 1A33
0561.05          ENDIF                                    AT 1A33
0562.04          IF(NORM.EQ.0) THEN                        AT 1A33
0563.05          B=DZERO                                  AT 1A40
0564.05          H=DZERO                                  AT 1A54
0565.05          D=DZERO                                  AT 1A68
0566.05          F=DZERO                                  AT 1A7C
0567.05          Z=DZERO                                  AT 1A90
0568.05          S=DZERO                                  AT 1AA4
0569.05          IF(I.NE.1) B=CC(IC)                     AT 1AB8
0570.05          IF(I.NE.NROW) H=CC(N)                   AT 1AE5
0571.05          IF(J.NE.1) D=CR(IR)                     AT 1B16
0572.05          IF(J.NE.NCOL) F=CR(N)                   AT 1B43
0573.05          IF(K.NE.1) Z=CV(IL)                     AT 1B74
0574.05          IF(K.NE.NLAY) S=CV(N)                   AT 1BA1
0575.05          HHCOF=HCOF(N) -Z-B-D-F-H-S             AT 1BD2
0576.05          ENDIF                                    AT 1C0D
0577.04          IF(NORM.EQ.1) HHCOF=-DONE               AT 1C0D
0578.04          CD(N)=(DONE+DEL)*HHCOF-CD CR-CDCC-CD CV-RELAX*(FCR+FCC+FCV) AT 1C2E
0579.04          IF(CD1.EQ.0.AND.CD(N).NE.0.) CD1=CD(N)  AT 1C7C
0580.04          C-----LT. CHANGED TO .LE. 01SEPT1991
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
0581.04          IF(CD(N)*CD1.LE.0.) THEN                 AT 1CBA
0582.04          C-----CHANGED 510 FORMAT 01SEPT1991 AND 20MAR1992
0583.04          C-----CHANGED 510 FORMAT AND WRITE STATEMENT AND ADDED DEL 01MAY1993
0584.05          DEL=1.5*DEL+.001                         AT 1CE0
0585.05          IF(DEL.GT.5) THEN                       AT 1CF9
0586.06          WRITE(IOUT,510)                         AT 1D09
0587.06          STOP                                     AT 1D2F
0588.06          ENDIF                                    AT 1D42
0589.05          GO TO 154                                AT 1D42
0590.05          ENDIF                                    AT 1D47
0591.04          ENDIF                                    AT 1D47
0592.03          510 FORMAT(' MATRIX IS SEVERELY NON-DAGONALLY DOMINANT. CHECK INPUT',
0593.03          1      ' FILES. STOP EXECUTION')
0594.03          C
0595.03          155 CONTINUE                             AT 1DAE
0596.03          C
0597.03          C-----STEP THROUGH EACH CELL AND SOLVE FOR S OF THE CONJUGATE
0598.03          C-----GRADIENT ALGORITHM BY BACK SUBSTITUTION. STORE RESULT IN SS.
0599          DO 160 KK=NLAY,1,-1                         AT 1DBD
0600.01          DO 160 II=NROW,1,-1                     AT 1DE0
0601.02          DO 160 JJ=NCOL,1,-1                     AT 1E03
0602.02          C
0603.03          N=JJ+(II-1)*NCOL+(KK-1)*NRC            AT 1E26
0604.03          IF(IBOUND(N).LE.0)GO TO 160            AT 1E4F
0605.03          C
0606.03          NC=N+1                                    AT 1E60
0607.03          NR=N+NCOL                                AT 1E67
0608.03          NL=N+NRC                                  AT 1E75
0609.03          SSCR=DZERO                                AT 1E87
0610.03          SSCC=DZERO                                AT 1E9B
0611.03          SSCV=DZERO                                AT 1EAF
0612.03          IF(JJ.NE.NCOL) SSCR=CR(N)*SS(NC)/CD(N) AT 1EC3
0613.03          IF(II.NE.NROW) SSCC=CC(N)*SS(NR)/CD(N) AT 1F08
0614.03          IF(KK.NE.NLAY) SSCV=CV(N)*SS(NL)/CD(N) AT 1F4A
0615.03          VN=V(N)/CD(N)                            AT 1F8C
0616.03          SS(N)=VN-SSCR-SSCC-SSCV                 AT 1FAD
0617.03          160 CONTINUE                             AT 1FCA
0618.03          C-----SKIP OVER OTHER PRECONDITIONING TYPES
0619          GO TO 199                                    AT 1FD9
0620          165 CONTINUE                                AT 1FDE
0621          C
0622          C-----POLYNOMIAL PRECONDITIONING
0623          DO 170 N=1,NODES                             AT 1FDE
0624.01          V(N)=RHS(N)                               AT 200B
0625.01          170 CONTINUE                             AT 2027
0626          CALL SPCG2E( IBOUND, RHS, HCOF, CR, CC, CV, V, SS, C2, NORM, NCOL, NROW,
0627          1          NLAY, NODES)                      AT 2029
0628          CALL SPCG2E( IBOUND, RHS, HCOF, CR, CC, CV, SS, V, C1, NORM, NCOL, NROW,
0629          1          NLAY, NODES)                      AT 207B
0630          CALL SPCG2E( IBOUND, RHS, HCOF, CR, CC, CV, V, SS, C0, NORM, NCOL, NROW,
0631          1          NLAY, NODES)                      AT 20CD

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0632      199 CONTINUE
0633      C
0634      C-----CALCULATE P OF THE CONJUGATE GRADIENT ALGORITHM
0635          SROLD=SRNEW
0636          SRNEW=DZERO
0637          DO 200 N=1,NODES
0638.01      IF (IBOUND(N) .LE.0) GO TO 200
0639.01      SRNEW=SRNEW+SS(N)*RHS(N)
0640.01      200 CONTINUE
0641.01      C
0642          IF (ITER.EQ.1) THEN
0643.01      DO 205 N=1,NODES
0644.02      205 P(N)=SS(N)
0645.01      ELSE
0646.01      DO 210 N=1,NODES
0647.02      210 P(N)=SS(N) + (SRNEW/SROLD)*P(N)
0648.01      ENDF
0649.01      C
0650.01      C-----CALCULATE ALPHA OF THE CONJUGATE GRADIENT ROUTINE.
0651.01      C-----FOR THE DENOMINATOR OF ALPHA, MULTIPLY THE MATRIX A BY THE
0652.01      C-----VECTOR P, AND STORE IN V; THEN MULTIPLY P BY V. STORE IN PAP.
0653          PAP=DZERO
0654          DO 290 K=1,NLAY
0655.01      DO 290 I=1,NROW
0656.02      DO 290 J=1,NCOL
0657.02      C
0658.03      N=J+ (I-1)*NCOL+ (K-1)*NRC
0659.03      V(N)=0.
0660.03      IF (IBOUND(N) .LE.0) GO TO 290
0661.03      C
0662.03      NRN=N+NCOL
0663.03      NRL=N-NCOL
0664.03      NCN=N+1
0665.03      NCL=N-1
0666.03      NLN=N+NRC
0667.03      NLL=N-NRC
0668.03      C
0669.03      NCF=N
0670.03      NCD=NCL
0671.03      NRB=NRL
0672.03      NRH=N
0673.03      NLS=N
0674.03      NLZ=NLL
0675.03      C
0676.03      B=DZERO
0677.03      IF (I.NE.1) B=CC(NRB)
0678.03      H=DZERO
0679.03      IF (I.NE.NROW) H=CC(NRH)
0680.03      D=DZERO
0681.03      IF (J.NE.1) D=CR(NCD)
0682.03      F=DZERO
0683.03      IF (J.NE.NCOL) F=CR(NCF)
0684.03      Z=DZERO
0685.03      IF (K.NE.1) Z=CV(NLZ)
0686.03      S=DZERO
0687.03      IF (K.NE.NLAY) S=CV(NLS)
0688.03      C
0689.03      IF (NORM.EQ.0) PN=P(N)
0690.03      IF (NORM.EQ.1) PN=DZERO
0691.03      BHNEW=DZERO
0692.03      HHNEW=DZERO
0693.03      DHNEW=DZERO
0694.03      FHNEW=DZERO
0695.03      ZHNEW=DZERO
0696.03      SHNEW=DZERO
0697.03      IF (NRL.GT.0) BHNEW=B*(P(NRL) - PN)
0698.03      IF (NRN.LE.NODES) HHNEW=H*(P(NRN) - PN)
0699.03      IF (NCL.GT.0) DHNEW=D*(P(NCL) - PN)
0700.03      IF (NCN.LE.NODES) FHNEW=F*(P(NCN) - PN)
0701.03      IF (NLL.GT.0) ZHNEW=Z*(P(NLL) - PN)
0702.03      IF (NLN.LE.NODES) SHNEW=S*(P(NLN) - PN)
0703.03      C
0704.03      C-----CALCULATE THE PRODUCT OF MATRIX A AND VECTOR P AND STORE
0705.03      C-----RESULT IN V.
0706.03      PN=HCOF(N)*P(N)
0707.03      IF (NORM.EQ.1) PN=-P(N)
0708.03      VN=ZHNEW+BHNEW+DHNEW+PN+FHNEW+HHNEW+SHNEW
0709.03      V(N)=VN
0710.03      PAP=PAP+P(N)*VN
0711.03      290 CONTINUE
0712.03      C
0713.03      C-----CALCULATE ALPHA

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0714          ALPHA=1.                                AT 280C
0715          IF(PAP.EQ.0..AND.MXITER.EQ.1) THEN      AT 2820
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
0716.01       WRITE(IOUT,520)                        AT 2842
0717.01       STOP                                  AT 2868
0718.01       ENDIF                                 AT 287B
0719          520   FORMAT(/,' CONJUGATE-GRADIENT METHOD FAILED.',/, ' SET MXITER',
0720             1   ' GREATER THAN ONE AND TRY AGAIN.  STOP EXECUTION')
0721          IF(PAP.NE.0.) ALPHA=SRNEW/PAP            AT 28FC
0722          C
0723          C-----CALCULATE NEW HEADS AND RESIDUALS, AND SAVE THE LARGEST
0724          C-----CHANGE IN HEAD AND THE LARGEST VALUE OF THE RESIDUAL.
WARNING - The use of .EQ. or .NE. with non-integer operands can produce misleading results
0725          DO 300 K=1,NLAY                          AT 2925
0726.01       DO 300 I=1,NROW                          AT 2952
0727.02       DO 300 J=1,NCOL                          AT 297F
0728.02       C
0729.03       N=J+(I-1)*NCOL+(K-1)*NRC                AT 29AC
0730.03       IF(IBOUND(N).LE.0) GO TO 300            AT 29D1
0731.03       C
0732.03       C-----HEAD
0733.03       HCHGN=ALPHA*P(N)                          AT 29E2
0734.03       IF(DABS(HCHGN).GT.ABS(BIGH)) THEN        AT 29F9
0735.04       BIGH=HCHGN                               AT 2A11
0736.04       IH=I                                     AT 2A29
0737.04       JH=J                                     AT 2A35
0738.04       KH=K                                     AT 2A41
0739.04       NH=N                                     AT 2A4D
0740.04       ENDIF                                    AT 2A53
0741.03       HNEW(N)=HNEW(N)+DAMP*HCHGN              AT 2A53
0742.03       C
0743.03       C-----RESIDUAL (V IS THE PRODUCT OF MATRIX A AND VECTOR P)
0744.03       RCHGN=-ALPHA*V(N)                          AT 2A73
0745.03       RHS(N)=RHS(N)+DAMP*RCHGN                 AT 2A8C
0746.03       IF(ABS(RHS(N)).GT.ABS(BIGR)) THEN        AT 2A9D
0747.04       BIGR=RHS(N)                              AT 2AB7
0748.04       IR=I                                     AT 2AD1
0749.04       JR=J                                     AT 2ADD
0750.04       KR=K                                     AT 2AE9
0751.04       NR=N                                     AT 2AF5
0752.04       ENDIF                                    AT 2AFB
0753.03       300 CONTINUE                             AT 2AFB
0754.03       C
0755.03       C-----UNSCALE LARGEST CHANGE IN HEAD AND LARGEST RESIDUAL, AND
0756.03       C-----CHECK THE CONVERGENCE CRITERION
0757          IF(NORM.EQ.1) THEN                        AT 2B0A
0758.01       BIGH=BIGH/SQRT(-HCOF(NH))                AT 2B17
0759.01       BIGR=BIGR/SQRT(-HCOF(NR))                AT 2B3A
0760.01       ENDIF                                    AT 2B55
0761          IF(MXITER.EQ.1) THEN                     AT 2B55
0762.01       IF(ABS(BIGH).LE.HCLOSE.AND.ABS(BIGR).LE.RCLOSE) ICNVG=1 AT 2B61
0763.01       ELSE                                    AT 2BA1
0764.01       IF(IITER.EQ.1.AND.
0765.01       1   ABS(BIGH).LE.HCLOSE.AND.ABS(BIGR).LE.RCLOSE) ICNVG=1 AT 2BA6
0766.01       ENDIF                                    AT 2BF3
0767          IF(ABS(BIGH).LE.HCLOSE.AND.ABS(BIGR).LE.RCLOSE) IICNVG=1 AT 2BF3
0768          C
0769          C-----STORE THE LARGEST UNSCALED HEAD CHANGE AND RESIDUAL VALUE
0770          C----- (THIS ITERATION) AND THEIR LOCATIONS.
0771          II=NITER                                   AT 2C31
0772          HCHG(II)=BIGH                             AT 2C3F
0773          LHCH(1,II)=KH                             AT 2C59
0774          LHCH(2,II)=IH                             AT 2C6E
0775          LHCH(3,II)=JH                             AT 2C85
0776          C
0777          RCHG(II)=BIGR                              AT 2C9C
0778          LRCH(1,II)=KR                             AT 2CBC
0779          LRCH(2,II)=IR                             AT 2CD1
0780          LRCH(3,II)=JR                             AT 2CE8
0781          C
0782          IT1(II)=0                                  AT 2CFF
0783          IF(IITER.EQ.1) IT1(II)=1                 AT 2D10
0784
0785          C-Environment Agency (UK)-12.Debugging output of unconverged heads>>>>>
0786          if(ipcgdebug.gt.0)then                     AT 2D25
0787          C-----copy HNEW to BUFF
0788.01       DO 311 N=1,NODES                          AT 2D31
0789.02       IF(NORM.EQ.1.and.IBOUND(N).ne.0) then    AT 2D5E
0790.03       HHCOF=SQRT(-HCOF(N))                    AT 2D7C
0791.03       buff(N)=HNEW(N)/HHCOF                   AT 2D91
0792.03       else                                     AT 2DA5
0793.03       buff(N)=HNEW(N)                          AT 2DAA

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0794.03          ENDIF                                     AT 2DC9
0795.02      311  CONTINUE                                 AT 2DC9
0796.02  C-----write heads to debug file
0797.01          IF (IXSEC.EQ.0) THEN                     AT 2DCE
0798.02              DO 79 K=1,NLAY                       AT 2DDA
0799.03                  KK=K                             AT 2E07
0800.03                      i=nrc*(k-1)+1               AT 2E0D
0801.03                      IF (CHEDFM.EQ.' ') THEN     AT 2E1C
0802.04                          CALL ULASAV(buff(i),TEXT,iiter,kiter,bigh,bigr,NCOL, AT 2E30
0803.04                              1                      NROW, KK, ipcgdebug)
0804.04                      ELSE                           AT 2E7E
0805.04                          CALL ULASV2(BUFF(i),TEXT,iiter,kiter,bigh,bigr,NCOL, AT 2E83
0806.04                              1                      NROW, KK, ipcgdebug, CHEDFM, LBHDSV, IBOUND(i))
0807.04                      END IF                         AT 2EE8
0808.03      79  CONTINUE                                 AT 2EE8
0809.02          ELSE                                     AT 2EED
0810.02              IF (CHEDFM.EQ.' ') THEN               AT 2EF2
0811.03                  CALL ULASAV(BUFF,TEXT,iiter,kiter,bigh,bigr,NCOL, AT 2F06
0812.03                      1                      NLAY,-1,ipcgdebug)
0813.03              ELSE                                   AT 2F47
0814.03                  CALL ULASV2(BUFF,TEXT,iiter,kiter,bigh,bigr,NCOL, AT 2F4C
0815.03                      1                      NLAY,-1,ipcgdebug,CHEDFM,LBHDSV,IBOUND)
0816.03              END IF                                 AT 2F9F
0817.02          END IF                                   AT 2F9F
0818.01      endif                                       AT 2F9F
0819.01  C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0820.01
0821.01  C-----GO TO NEXT INTERNAL ITERATION IF CONVERGENCE HAS NOT BEEN
0822.01  C-----REACHED AND IITER IS LESS THAN ITER1
0823          IF (MXITER.EQ.1) THEN                         AT 2F9F
0824.01              IF (ICNVG.EQ.0.AND.IITER.LT.ITER1) GO TO 153 AT 2FAB
0825.01          ELSE                                       AT 2FCB
0826.01              IF (IICNVG.EQ.0.AND.IITER.LT.ITER1) GO TO 153 AT 2FD0
0827.01          ENDIF                                       AT 2FEE
0828.01  C
0829.01  C-----UNSCALE CR,CC,CV AND HNEW
0830          IF (NORM.EQ.1) THEN                             AT 2FEE
0831.01              DO 310 N=1,NODES                         AT 2FFB
0832.02              IF (IBOUND(N).EQ.0) GO TO 310          AT 3028
0833.02              HHCOF=SQRT(-HCOF(N))                   AT 3039
0834.02              IF (N.LE.(NODES-NCOL).AND.CC(N).GT.0.) AT 304E
0835.02              #   CC(N)=CC(N)*(HHCOF*(SQRT(-HCOF(N+NCOL))))
0836.02              IF (N.LE.(NODES-1).AND.CR(N).GT.0.)    AT 30A3
0837.02              #   CR(N)=CR(N)*(HHCOF*(SQRT(-HCOF(N+1))))
0838.02              IF (N.LE.(NODES-NRC).AND.CV(N).GT.0.) AT 30F8
0839.02              #   CV(N)=CV(N)*(HHCOF*(SQRT(-HCOF(N+NRC))))
0840.02              HNEW(N)=HNEW(N)/HHCOF                   AT 315E
0841.02      310  CONTINUE                                 AT 3179
0842.01          ENDIF                                       AT 317E
0843.01  C
0844.01  C-Environment Agency (UK)-11.Force converge if NOUTC outer itr conv>>>>
0845          IF (MXITER.ne.1.and.IICNVG.EQ.1) nout=nout+1 AT 317E
0846          if (nout.eq.noutc.and.noutc.ne.0) then        AT 319C
0847.01              write(IOUT,503)nout                     AT 31B5
0848.01              ICNVG=1                                  AT 31EB
0849.01          endif                                       AT 31F7
0850      503  format(' PCG2 CONVERGENCE STOPPED AFTER',i6,' CONSECUTIVE OUTER ' AT 31F7
0851          1          , 'ITERATIONS WITH ERROR CRITERIA ACHIEVED.'/
0852          2          , ' CAREFULLY LOOK AT MASS BALANCE TO VALIDATE RESULTS.')
0853  C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0854  C
0855  C-----IF END OF TIME STEP, PRINT # OF ITERATIONS THIS STEP
0856          IF (ICNVG.EQ.0 .AND. KITER.NE.MXITER) GO TO 600 AT 32B0
0857          IF (MUTPCG.GT.1) GO TO 590                     AT 32D2
0858          IF (KSTP.EQ.1) WRITE(IOUT,500)                 AT 32DE
0859      500  FORMAT(1H0)                                     AT 3313
0860          WRITE(IOUT,501) KITER,KSTP,KPER,NITER         AT 3328
0861      501  FORMAT(1X,I5,' CALLS TO PCG ROUTINE FOR TIME STEP',I4, AT 339A
0862          1' IN STRESS PERIOD',I3,/1X,I5,' TOTAL ITERATIONS')
0863          IF (MUTPCG.EQ.1) GO TO 590                     AT 3421
0864  C
0865  C-----PRINT HEAD CHANGE EACH ITERATION IF PRINTOUT INTERVAL IS REACHED
0866          IF (ICNVG.EQ.0 .OR. KSTP.EQ.NSTP .OR. MOD(KSTP,IPRPCG).EQ.0) AT 342D
0867          1          CALL SPCG2P(HCHG,LHCH,RCHG,LRCH,
0868          2          ITER1,NITER,MXITER,IOUT,NPCOND,BPOLY,IT1)
0869  C-Environment Agency (UK)-10.Convergence info output to screen>>>>>>>>>>>>
0870  c590  NITER=0
0871      590  write(*,502) KPER,KSTP,NITER,HCHG(NITER),RCHG(NITER) AT 349C
0872      502  format(' |',i7,' |',i5,' |',i6,' |',g11.4,' |',g11.4,' |') AT 353D
0873          NITER=0                                         AT 3592
0874  C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0875  C

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0876      C-----RETURN
0877      600  RETURN
0878      C
0879      END
WARNING - Label 895 has not been referenced
WARNING - Label 900 has not been referenced

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0880      SUBROUTINE SPCG2P(HCHG,LHCH,RCHG,LRCH,ITER1,
0881      1          NITER,MXITER,IOUT,NPCOND,BPOLY,IT1)
0882      C
0883      C
0884      C-----VERSION 0001 01MAY1988 SPCG2P
0885      C *****
0886      C PRINT MAXIMUM HEAD CHANGE AND RESIDUAL VALUE FOR EACH ITERATION
0887      C DURING A TIME STEP
0888      C *****
0889      C
0890      C SPECIFICATIONS:
0891      C -----
0892      C
0893      C DIMENSION HCHG(MXITER*ITER1), LHCH(3,MXITER*ITER1)
0894      C DIMENSION RCHG(MXITER*ITER1), LRCH(3,MXITER*ITER1)
0895      C DIMENSION IT1(MXITER*ITER1)
0896      C -----
0897      C
0898      C IF(NPCOND.EQ.2) WRITE(IOUT,2) BPOLY
0899      2 FORMAT(1H0,'B OF THE POLYNOMIAL PRECONDITIONING METHOD: ',E12.4)
0900      WRITE(IOUT,5)
0901      5 FORMAT(1H0,'MAXIMUM HEAD CHANGE FOR EACH ITERATION (1 INDICATES ',
0902      A 'THE FIRST INNER ITERATION):'/
0903      1 1H0,4(' HEAD CHANGE LAYER,ROW,COL')/1X,120('-'))
0904      WRITE(IOUT,10) (IT1(J),HCHG(J),(LHCH(I,J),I=1,3),J=1,NITER)
0905      WRITE(IOUT,11)
0906      WRITE(IOUT,15)
0907      15 FORMAT(1H0,'MAXIMUM RESIDUAL FOR EACH ITERATION (1 INDICATES ',
0908      A 'THE FIRST INNER ITERATION):'/
0909      1 1H0,4(' RESIDUAL LAYER,ROW,COL')/1X,120('-'))
0910      WRITE(IOUT,10) (IT1(J),RCHG(J),(LRCH(I,J),I=1,3),J=1,NITER)
0911      WRITE(IOUT,11)
0912      C
0913      C RETURN
0914      C
0915      10 FORMAT((1X,4(2X,I1,1X,G12.4,' (' ,I3,',',I3,',',I3,')'))
0916      11 FORMAT(1H0)
0917      C
0918      C END

```

```

AT 359E
AT 35A3
AT 0033
AT 0075
AT 00C2
AT 00E8
AT 01A3
AT 024E
AT 0274
AT 029A
AT 0353
AT 03FE
AT 0424
AT 0429
AT 0490
AT 04A5

```

```

0919      SUBROUTINE SPCG2E(IBOUND,RHS,HCOF,CR,CC,CV,VIN,VOUT,C,NORM,NCOL,
0920      1          NROW,NLAY,NODES)
0921      C
0922      C
0923      C-----VERSION 0001 01MAY1989 SPCG2E
0924      C *****
0925      C MATRIX MULTIPLICATIONS FOR POLYNOMIAL PRECONDITIONING
0926      C *****
0927      C
0928      C SPECIFICATIONS:
0929      C -----
0930      C
0931      C DOUBLE PRECISION VN,CRHS,Z,B,D,F,H,S,ZV,BV,DV,FV,HV,SV,DZERO
0932      C DIMENSION IBOUND(NODES),CR(NODES),CC(NODES),CV(NODES),
0933      1 RHS(NODES),VIN(NODES),VOUT(NODES),HCOF(NODES)
0934      C -----
0935      C
0936      C DZERO=0.
0937      C NRC=NROW*NCOL
0938      C DO 290 K=1,NLAY
0939      01 DO 290 I=1,NROW
0940      02 DO 290 J=1,NCOL
0941      02 C
0942      03 N=J+(I-1)*NCOL+(K-1)*NRC
0943      03 VOUT(N)=0.
0944      03 IF(IBOUND(N).LE.0)GO TO 290
0945      03 C
0946      03 NRN=N+NCOL
0947      03 NRL=N-NCOL
0948      03 NCN=N+1
0949      03 NCL=N-1

```

```

AT 0026
AT 0034
AT 0042
AT 0060
AT 007E
AT 009C
AT 00B5
AT 00C8
AT 00D6
AT 00DB
AT 00E6
AT 00F0

```

```

0950.03      NLN=N+NRC                                AT 00FA
0951.03      NLL=N-NRC                                AT 0106
0952.03      C
0953.03      NCF=N                                    AT 0112
0954.03      NCD=NCL                                  AT 011B
0955.03      NRB=NRL                                  AT 0127
0956.03      NRH=N                                    AT 0133
0957.03      NLS=N                                    AT 013C
0958.03      NLZ=NLL                                  AT 0142
0959.03      C
0960.03      B=DZERO                                  AT 014E
0961.03      BV=DZERO                                  AT 0160
0962.03      IF (I.NE.1.AND.IBOUND(NRL).GE.0) THEN    AT 0172
0963.03          B=CC(NRB)                             AT 018D
0964.03          BV=B*VIN(NRL)                         AT 01AA
0965.03      ENDIF                                    AT 01C4
0966.03      H=DZERO                                  AT 01C4
0967.03      HV=DZERO                                  AT 01D6
0968.03      IF (I.NE.NROW.AND.IBOUND(NRN).GE.0) THEN AT 01E8
0969.03          H=CC(NRH)                             AT 0207
0970.03          HV=H*VIN(NRN)                         AT 0224
0971.03      ENDIF                                    AT 023B
0972.03      D=DZERO                                  AT 023B
0973.03      DV=DZERO                                  AT 024D
0974.03      IF (J.NE.1.AND.IBOUND(NCL).GE.0) THEN    AT 025F
0975.03          D=CR(NCD)                             AT 027D
0976.03          DV=D*VIN(NCL)                         AT 029A
0977.03      ENDIF                                    AT 02B4
0978.03      F=DZERO                                  AT 02B4
0979.03      FV=DZERO                                 AT 02C6
0980.03      IF (J.NE.NCOL.AND.IBOUND(NCN).GE.0) THEN AT 02D8
0981.03          F=CR(NCF)                             AT 02FA
0982.03          FV=F*VIN(NCN)                         AT 0317
0983.03      ENDIF                                    AT 0331
0984.03      Z=DZERO                                  AT 0331
0985.03      ZV=DZERO                                  AT 0343
0986.03      C    IF STATEMENT REARRANGED 01JUN1993
0987.03      IF (K.NE.1) THEN                          AT 0355
0988.03          IF (IBOUND(NLL).GE.0) THEN            AT 035F
0989.03              Z=CV(NLZ)                         AT 0373
0990.03              ZV=Z*VIN(NLL)                    AT 0390
0991.03          ENDIF                                  AT 03AA
0992.03      ENDIF                                    AT 03AA
0993.03      S=DZERO                                  AT 03AA
0994.03      SV=DZERO                                  AT 03BC
0995.03      IF (K.NE.NLAY.AND.IBOUND(NLN).GE.0) THEN AT 03CE
0996.03          S=CV(NLS)                             AT 03F0
0997.03          SV=S*VIN(NLN)                        AT 040D
0998.03      ENDIF                                    AT 0427
0999.03      C
1000.03      C-----CALCULATE THE PRODUCT OF MATRIX A AND VECTOR VIN AND STORE
1001.03      C----- RESULT IN VOUT
1002.03          VN=HCOF(N)*VIN(N)                     AT 0427
1003.03          IF (NORM.EQ.1) VN=-VIN(N)             AT 043F
1004.03          CRHS=C*RHS(N)                         AT 0458
1005.03          VOUT(N)=CRHS+ZV+B*VIN(N)+DV+VN+FV+HV+SV AT 046E
1006.03      290 CONTINUE
1007          RETURN                                    AT 04AF
1008          END                                        AT 04B4

```

End of compilation - Clocked 0.0 seconds

APPENDIX D
Modified computer code for MODFLOW utilities package
with changes highlighted

COMPILER OPTIONS: listing intl no_persist nodclvar nomap nocheck logl dynm offset dreal noansi
 nopagethrow

nosilent no_optimise warn73 nolink no_link

```

0001 C-Changes to the code are highlighted with the following headings:
0002 C
0003 C-Environment Agency (UK)-9.Allow direct access binary output files>>>>
0004 C-Environment Agency (UK)-10.Allow double precn dir access bin output>>>
0005 C
0006 C These headings are followed by the original USGS MODFLOW-96 code
0007 C (commented out), followed by the modified code. All the code changes
0008 C are followed by the following:
0009 C
0010 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0011 C
0012 SUBROUTINE UBUDSV(KSTP,KPER,TEXT,IBDCHN,BUFF,NCOL,NROW,NLAY,IOUT)
0013 C
0014 C
0015 C-----VERSION 1039 26JUNE1992 UBUDSV
0016 C *****
0017 C RECORD CELL-BY-CELL FLOW TERMS FOR ONE COMPONENT OF FLOW.
0018 C *****
0019 C
0020 C SPECIFICATIONS:
0021 C -----
0022 C-Environment Agency (UK)-9.Allow direct access binary output files>>>>
0023 c CHARACTER*16 TEXT
0024 c DIMENSION BUFF(NCOL,NROW,NLAY)
0025 character text*4,acc*10
0026 DIMENSION BUFF(NCOL,NROW,NLAY),text(4)
0027 character fname*100
0028 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0029 C -----
0030 C
0031 C1-----WRITE AN UNFORMATTED RECORD IDENTIFYING DATA.
0032 WRITE(IOUT,1) TEXT,IBDCHN,KSTP,KPER AT 004C
0033 C-Environment Agency (UK)-9.Allow direct access binary output files>>>>
0034 c 1 FORMAT(1X,'UBUDSV SAVING ',A16,' ON UNIT',I3,
0035 c 1 ' AT TIME STEP',I3,', STRESS PERIOD',I3)
0036 1 FORMAT(1X,'UBUDSV SAVING ',A4,' ON UNIT',I3, AT 00B8
0037 1 ' AT TIME STEP',I3,', STRESS PERIOD',I3)
0038 c
0039 c1a-----CHECK ACCESS OF FILE
0040 inquire(ibdchn,access=acc) AT 012B
0041 if(acc.eq.'DIRECT')then AT 014F
0042.01 inquire(ibdchn,recl=irecl,nextrec=nr) AT 0165
0043.01 if(nr.eq.1)then AT 018C
0044.02 inquire(ibdchn,name=fname) AT 0196
0045.02 close(ibdchn,status='delete') AT 01BD
0046.02 C-Environment Agency (UK)-10.Allow double precn dir access bin output>>>
0047.02 c irecl=((ncol*nrow*nlay)+9)*4
0048.02 irecl=((ncol*nrow*nlay*2)+9)*4 AT 01E2
0049.02 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0050.02 open(ibdchn,file=fname,access='direct',recl=irecl) AT 01FE
0051.02 endif AT 023E
0052.01 write(ibdchn,rec=nr)KSTP,KPER,TEXT,NCOL,NROW,NLAY, AT 023E
0053.01 1 ((BUFF(IC,IR,il),IC=1,NCOL),IR=1,NROW),il=1,nlay)
0054.01 goto 999 AT 03B1
0055.01 endif AT 03B6
0056.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0057 WRITE(IBDCHN) KSTP,KPER,TEXT,NCOL,NROW,NLAY AT 03B6
0058 C
0059 C2-----WRITE AN UNFORMATTED RECORD CONTAINING VALUES FOR
0060 C2-----EACH CELL IN THE GRID.
0061 WRITE(IBDCHN) BUFF AT 0454
0062 C
0063 C-Environment Agency (UK)-9.Allow direct access binary output files>>>>
0064 999 continue AT 0482
0065 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0066 C3-----RETURN
0067 RETURN AT 0482
0068 END AT 0487

0442 SUBROUTINE ULASAV(BUF,TEXT,KSTP,KPER,PERTIM,TOTIM,NCOL,
0443 1 NROW,ILAY,ICHN)
0444 C
0445 C-----VERSION 1642 12MAY1987 ULASAV
    
```

```

0446 C *****
0447 C SAVE 1 LAYER ARRAY ON DISK
0448 C *****
0449 C
0450 C SPECIFICATIONS:
0451 C -----
0452 CHARACTER*4 TEXT
0453 DIMENSION BUF(NCOL,NROW),TEXT(4)
0454 C-Environment Agency (UK)-9.Allow direct access binary output files>>>>
0455 character*10 ACC
0456 character fname*100
0457 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0458 C -----
0459 C-Environment Agency (UK)-9.Allow direct access binary output files>>>>
0460 c0-----CHECK ACCESS OF HEADS FILE
0461 inquire(ichn,access=acc) AT 003B
0462 if(acc.eq.'DIRECT')then AT 005F
0463.01 inquire(ichn,recl=irecl,nextrec=nr) AT 0075
0464.01 if(nr.eq.1)then AT 009C
0465.02 inquire(ichn,name=fname) AT 00A6
0466.02 close(ichn,status='delete') AT 00CD
0467.02 C-Environment Agency (UK)-10.Allow double precn dir access bin output>>>
0468.02 c irecl=((ncol*nrow)+11)*4
0469.02 irecl=((ncol*nrow*2)+13)*4 AT 00F2
0470.02 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0471.02 open(ichn,file=fname,access='direct',recl=irecl) AT 0108
0472.02 endif AT 0148
0473.01 write(ichn,rec=nr)KSTP,KPER,PERTIM,TOTIM,TEXT,NCOL,NROW,ILAY, AT 0148
0474.01 1 ((BUF(IC,IR),IC=1,NCOL),IR=1,NROW)
0475.01 goto 999 AT 02A6
0476.01 endif AT 02AB
0477.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0478.01 C
0479.01 C1-----WRITE AN UNFORMATTED RECORD CONTAINING IDENTIFYING
0480.01 C1-----INFORMATION.
0481 WRITE(ICHN) KSTP,KPER,PERTIM,TOTIM,TEXT,NCOL,NROW,ILAY AT 02AB
0482 C
0483 C2-----WRITE AN UNFORMATTED RECORD CONTAINING ARRAY VALUES
0484 C2-----THE ARRAY IS DIMENSIONED (NCOL,NROW)
0485 WRITE(ICHN) ((BUF(IC,IR),IC=1,NCOL),IR=1,NROW) AT 0373
0486 C
0487 C-Environment Agency (UK)-9.Allow direct access binary output files>>>>
0488 999 continue AT 041A
0489 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0490 C3-----RETURN
0491 RETURN AT 041A
0492 END AT 041F

```

APPENDIX E
Modified computer code for main MODFLOW program
with changes highlighted

COMPILER OPTIONS: listing intl no_persist nodclvar nomap nocheck logl dynm offset dreal noansi
nopagethrow

nosilent no_optimise warn73 nolink no_link

```
0001 C *****
0002 C MODFLOW-VKD Version 3 (14 MAY 2003)
0003 C     MODIFIED TO INCLUDE VARIATIONS IN HYDRAULIC CONDUCTIVITY AND
0004 C     STORAGE WITH DEPTH.
0005 C     BY THE ENVIRONMENT AGENCY (UK) & WATER MANAGEMENT
0006 C     CONSULTANTS LTD. - A. Taylor, P. Hulme and A. Hughes
0007 C MODFLOW-VKD Version 1 documented in:
0008 C     Environment Agency, 2002a, Enhancements to MODFLOW -
0009 C     Variation in hydraulic conductivity and storage with depth.
0010 C     WMC Report 1621/R1 prepared for the Environment Agency,
0011 C     National Groundwater and Contaminated Land Centre,
0012 C     Project NC/00/23.
0013 C     and
0014 C     Environment Agency, 2002b, Enhancements to MODFLOW -
0015 C     User guide for MODFLOW-VKD - A modified version of
0016 C     MODFLOW-96 to include variations in hydraulic properties
0017 C     with depth. WMC Report 1621/R2 prepared for the Environment
0018 C     Agency, National Groundwater and Contaminated Land Centre,
0019 C     Project NC/00/23.
0020 C
0021 C-Changes to the code are highlighted with the following headings:
0022 C
0023 C-Environment Agency (UK)-0.General change to enable new options>>>>>>
0024 C-Environment Agency (UK)-1.Variable hydraulic cond. w/depth (VKD)>>>>>>
0025 C-Environment Agency (UK)-2.Variable storage with depth (VSD)>>>>>>>>
0026 C-Environment Agency (UK)-3.Auto-conversion for steady state VKD>>>>>>
0027 C-Environment Agency (UK)-4.Spatially variable anisotropy>>>>>>>>>>
0028 C-Environment Agency (UK)-5.Inter-nodal transmissivities>>>>>>>>>>
0029 C-Environment Agency (UK)-6.X & Y-dir transmissivities>>>>>>>>>>>>
0030 C-Environment Agency (UK)-7.Explicit transmissivity calculation>>>>>>>>
0031 C-Environment Agency (UK)-8.Output calculated transmissivities>>>>>>>>
0032 C-Environment Agency (UK)-9.Allow direct access binary output files>>>>>
0033 C-Environment Agency (UK)-10.Convergence info output to screen>>>>>>>>
0034 C-Environment Agency (UK)-11.Force converge if NOUTC outer itrs conv>>>>
0035 C-Environment Agency (UK)-12.Debugging output of unconverged heads>>>>>
0036 C-Environment Agency (UK)-13.Allow an inflow to any stream reach>>>>>>>
0037 C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>>
0038 C-Environment Agency (UK)-15.Save single flow if >1 stream in a cell>>>>
0039 C-Environment Agency (UK)-16.K gradient independant of kbase>>>>>>>>>>
0040 C-Environment Agency (UK)-17.Output calc trans to binary file>>>>>>>>>>
0041 C
0042 C These headings are followed by the original USGS MODFLOW-96 code
0043 C (commented out), followed by the modified code. All the code changes
0044 C are followed by the following:
0045 C
0046 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0047 C
0048 C-Based on USGS:
0049 C *****
0050 C     MAIN CODE FOR U.S. GEOLOGICAL SURVEY MODULAR MODEL -- MODFLOW-96
0051 C     BY MICHAEL G. MCDONALD AND ARLEN W. HARBAUGH
0052 C     MODFLOW-88 documented in:
0053 C     McDonald, M.G. and Harbaugh, A.W., 1988, A modular
0054 C     three-dimensional finite-difference ground-water flow
0055 C     model: U.S. Geological Survey Techniques of Water
0056 C     Resources Investigations, Book 6, Chapter A1, 586 p.
0057 C     MODFLOW-96 documented in:
0058 C     Harbaugh, A.W. and McDonald, M.G., 1996, User's
0059 C     documentation for the U.S. Geological Survey modular
0060 C     finite-difference ground-water flow model: U.S. Geological
0061 C     Survey Open-File Report 96-485
0062 C-----VERSION 0950 23MAY1996 MAIN
0063 C-----VERSION 1401 03DEC1996 -- added PCG2, STR1, IBS1, CHD1, GFD1,
0064 C     HFB1, TLK1, DE45, and RES1 as documented
0065 C     in USGS reports
0066 C *****
0067 C
0068 C     SPECIFICATIONS:
0069 C     -----
0070 C1-----SPECIFY THE SIZE OF THE X ARRAY. TO CHANGE THE SIZE OF THE
0071 C1-----X ARRAY, CHANGE VALUE OF LENX IN THE NEXT STATEMENT.
0072 C-Environment Agency (UK)-0.General change to enable new options>>>>>>
0073 C     PARAMETER (LENX=1500000)
0074 C     PARAMETER (LENX=10000000)
0075 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
```

```

0076      COMMON X(LENX)
0077      COMMON /FLWCOM/LAYCON(200)
0078      CHARACTER*16 VBNM(40)
0079      CHARACTER*80 HEADNG(2)
0080      DIMENSION VBVL(4,40),IUNIT(40)
0081      DOUBLE PRECISION DUMMY
0082      EQUIVALENCE (DUMMY,X(1))
0083      CHARACTER*20 CHEDFM,CDDNFM
0084      CHARACTER*80 FNAME
0085      C-Environment Agency (UK)-3.Auto-conversion for steady state VKD>>>>>>>>
0086      logical exists2
0087      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0088      LOGICAL EXISTS
0089      CHARACTER*4 CUNIT(40)
0090      DATA CUNIT/'BCF ','WEL ','DRN ','RIV ','EVT ','TLK ','GHB ','
0091      1          'RCH ','SIP ','DE4 ','SOR ','OC ','PCG ','GFD ','
0092      2          'HFB ','RES ','STR ','IBS ','CHD ','FHB ','
0093      3          ' ',' ',' ',' ',' ',' ',' ',' ',' ',' ',' ','
0094      4          ' ',' ',' ',' ',' ',' ',' ',' ',' ',' ',' ','
0095      5          ' ',' ',' ',' ',' ',' ',' ',' ',' ',' ',' '
0096      C
0097      C
0098      set string for use if RCS ident command
0099      FNAME =
0100      &'$Id: modflow96.f,v 3.2 1998/01/09 19:19:39 rsregan Exp rsregan $'
0101      FNAME =
0102      &'@(#)MODFLOW-96 - Modular 3-D Finite-Difference GW Flow Model'
0103      FNAME = '@(#)MODFLOW-96 - USGS TWRI, Book 6, Chap. A1, McDonald an
0104      &d Harbaugh'
0105      FNAME = '@(#)MODFLOW-96 - USGS OFR 96-485, Harbaugh and McDonald'
0106      FNAME =
0107      &'@(#)MODFLOW-96 - Contact: h2osoft@usgs.gov'
0108      FNAME = '@(#)MODFLOW-96 - Version: 3.0 1996/12/03 includes MOC'
0109      FNAME =
0110      &'@(#)MODFLOW-96 - Version: 3.1 1997/03/11 fixed HFBIFM call'
0111      FNAME = '@(#)MODFLOW-96 - Version: 3.2x 1998/01/09 includes FHB'
0112      C-Environment Agency (UK)-0.General change to enable new options>>>>>>>>
0113      FNAME = '@(#)MODFLOW-VKD - Version: 1.0 18/07/2001 includes VKD'
0114      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0115      C
0116      INUNIT=99
0117      IBUNIT=98
0118      IBOUTS=97
0119      C-Environment Agency (UK)-3.Auto-conversion for steady state VKD>>>>>>>>
0120      ibcfoutunit=96
0121      inoutunit=95
0122      ioutbas=94
0123      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0124      IBATCH=0
0125      INQUIRE(FILE='modflow.bf',EXIST=EXISTS)
0126      IF(EXISTS) THEN
0127      IBATCH=1
0128      OPEN(UNIT=IBUNIT,FILE='modflow.bf',STATUS='OLD')
0129      OPEN(UNIT=IBOUTS,FILE='modbatch.rpt')
0130      WRITE(IBOUTS,*) ' USGS MODFLOW MODEL BATCH-MODE REPORT'
0131      END IF
0132      C
0133      C2-----OPEN FILE OF FILE NAMES.
0134      50 IF(IBATCH.GT.0) THEN
0135      READ(IBUNIT,'(A)',END=500) FNAME
0136      IF(FNAME.EQ.' ') GO TO 50
0137      WRITE(IBOUTS,'(1X,/1X,A)') FNAME
0138      ELSE
0139      WRITE(*,*) ' Enter the name of the NAME FILE:'
0140      READ(*,'(A)') FNAME
0141      END IF
0142      INQUIRE(FILE=FNAME,EXIST=EXISTS)
0143      IF(.NOT.EXISTS) THEN
0144      IF(IBATCH.GT.0) THEN
0145      WRITE(IBOUTS,*) ' Specified name file does not exist.'
0146      WRITE(IBOUTS,*) ' Processing will continue with the next ',
0147      'name file in modflow.bf.'
0148      ELSE
0149      WRITE(*,*) ' File does not exist'
0150      END IF
0151      GO TO 50
0152      END IF
0153      C-Environment Agency (UK)-3.Auto-conversion for steady state VKD>>>>>>>>
0154      c OPEN(UNIT=INUNIT,FILE=FNAME,STATUS='OLD')
0155      55 OPEN(UNIT=INUNIT,FILE=FNAME,STATUS='OLD')
0156      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0157      C
0158      C3-----DEFINE PROBLEM--ROWS,COLUMNS,LAYERS,STRESS PERIODS,PACKAGES.

```

```

0158          CALL BAS5DF (ISUM,HEADNG,NPER,ITMUNI,TOTIM,NCOL,NROW,NLAY,
0159          1          NODES,INBAS,IOUT,IUNIT,CUNIT,INUNIT,IXSEC,ICHFLG,IFREFM)
0160          C
0161          C4-----ALLOCATE SPACE IN "X" ARRAY.
0162          CALL BAS5AL (ISUM,LENX,LCHNEW,LCHOLD,LCIBOU,LCCR,LCCC,LCCV,
0163          1          LCHCOF,LCRHS,LCDELR,LCDELCLC,LCSTRT,LCBUFF,LCIOFL,
0164          2          INBAS,ISTRN,NCOL,NROW,NLAY,IOUT,IAPART,IFREFM)
0165          C-Environment Agency (UK)-0.General change to enable new options>>>>>>>>
0166          c          IF (IUNIT(1).GT.0) CALL BCF5AL (ISUM,LENX,LCSC1,LCHY,
0167          c          1          LCBOT,LCTOP,LCSC2,LCTRPY,IUNIT(1),ISS,
0168          c          2          NCOL,NROW,NLAY,IOUT,IBCFB,LCWETD,IWDFLG,LCCVWD,
0169          c          3          WETFCT,IWETIT,IHDWET,HDRY,IAPART,IFREFM)
0170          C-Environment Agency (UK)-16.K gradient independant of kbase>>>>>>>>>>>>
0171          c          IF (IUNIT(1).GT.0) CALL BCF5AL (ISUM,LENX,LCSC1,LCHY,
0172          c          1          LCBOT,LCTOP,LCSC2,LCTRPY,IUNIT(1),ISS,
0173          c          2          NCOL,NROW,NLAY,IOUT,IBCFB,LCWETD,IWDFLG,LCCVWD,
0174          c          3          WETFCT,IWETIT,IHDWET,HDRY,IAPART,IFREFM,itrpy,lckgrad,ihold,
0175          c          4          itrans,lcmid,lckmax,lcsgrad,lcsmax,lcsmid)
0176          IF (IUNIT(1).GT.0) CALL BCF5AL (ISUM,LENX,LCSC1,LCHY,
0177          1          LCBOT,LCTOP,LCSC2,LCTRPY,IUNIT(1),ISS,
0178          2          NCOL,NROW,NLAY,IOUT,IBCFB,LCWETD,IWDFLG,LCCVWD,
0179          3          WETFCT,IWETIT,IHDWET,HDRY,IAPART,IFREFM,itrpy,lckgrad,ihold,
0180          4          itrans,lcmid,lckmax,lcsgrad,lcsmax,lcsmid,ikbase)
0181          C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0182          C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0183          IF (IUNIT(2).GT.0) CALL WEL5AL (ISUM,LENX,LCWELL,MXWELL,NWELLS,
0184          1          IUNIT(2),IOUT,IWELCB,NWELVL,IWELAL,IFREFM)
0185          IF (IUNIT(3).GT.0) CALL DRN5AL (ISUM,LENX,LCDRAI,NDRAIN,MXDRN,
0186          1          IUNIT(3),IOUT,IDRNCB,NDRNVL,IDRNAL,IFREFM)
0187          IF (IUNIT(4).GT.0) CALL RIV5AL (ISUM,LENX,LCRIVR,MXRIVR,NRIVER,
0188          1          IUNIT(4),IOUT,IRIVCB,NRIVVL,IRIVAL,IFREFM)
0189          IF (IUNIT(5).GT.0) CALL EVT5AL (ISUM,LENX,LCIEVT,LCEVTR,LCEXDP,
0190          1          LCSURF,NCOL,NROW,NEVTOP,IUNIT(5),IOUT,IEVTCB,IFREFM)
0191          IF (IUNIT(6).GT.0) CALL TLK1AL (ISUM,LENX,NCOL,NROW,NLAY,
0192          1          LCRAT,LCZCB,LCA1,LCB1,LCALPH,LCBET,LCRM1,LCRM2,LCRM3,
0193          2          LCRM4,LCTL,LCTLK,LCSLU,LCSLD,NODES1,NM1,NM2,NUMC,
0194          3          NTM1,ITLKS,ITLKR,ITLKB,ISS,IUNIT(6),IOUT)
0195          IF (IUNIT(7).GT.0) CALL GHB5AL (ISUM,LENX,LCBND,NBOUND,MXBND,
0196          1          IUNIT(7),IOUT,IGHBCB,NGHBVL,IGHBAL,IFREFM)
0197          IF (IUNIT(8).GT.0) CALL RCH5AL (ISUM,LENX,LCIRCH,LCRECH,NRCHOP,
0198          1          NCOL,NROW,IUNIT(8),IOUT,IRCHCB,IFREFM)
0199          IF (IUNIT(9).GT.0) CALL SIP5AL (ISUM,LENX,LCEL,LCFL,LCGL,LCV,
0200          1          LCHDCG,LCLRCH,LCW,MXITER,NPARN,NCOL,NROW,NLAY,
0201          2          IUNIT(9),IOUT,IFREFM)
0202          IF (IUNIT(10).GT.0) CALL DE45AL (ISUM,LENX,LCAU,LCAL,LCIUPP,
0203          1          LCIEQP,LCD4B,LCLRCH,LCHDCG,
0204          2          MXUP,MXLOW,MXEQ,MXBW,IUNIT(10),ITMX,ID4DIR,
0205          3          NCOL,NROW,NLAY,IOUT,ID4DIM)
0206          IF (IUNIT(11).GT.0) CALL SORSAL (ISUM,LENX,LCA,LCRES,LCHDCG,LCLRCH,
0207          1          LCIEQP,MXITER,NCOL,NLAY,NSLICE,MBW,IUNIT(11),IOUT,IFREFM)
0208          C-Environment Agency (UK)-0.General change to enable new options>>>>>>>>
0209          c          IF (IUNIT(13).GT.0) CALL PCG2AL (ISUM,LENX,LCV,LCSS,LCP,LCCD,
0210          c          1          LCHCHG,LCLHCH,LCRCHG,LCLRCH,MXITER,ITER1,NCOL,NROW,NLAY,
0211          c          2          IUNIT(13),IOUT,NPCOND,LCIT1)
0212          IF (IUNIT(13).GT.0) CALL PCG2AL (ISUM,LENX,LCV,LCSS,LCP,LCCD,
0213          1          LCHCHG,LCLHCH,LCRCHG,LCLRCH,MXITER,ITER1,NCOL,NROW,NLAY,
0214          2          IUNIT(13),IOUT,NPCOND,LCIT1,noutc,ipcgdebug,iapart)
0215          C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0216          IF (IUNIT(14).GT.0) CALL GFD1AL (ISUM,LENX,LCSC1,LCCDTR,LCCDTC,
0217          1          LCBOT,LCTOP,LCSC2,IUNIT(14),ISS,NCOL,NROW,NLAY,IOUT,IGFDCB)
0218          IF (IUNIT(16).GT.0) CALL HFB1AL (ISUM,LENX,LCHFBR,NHFB,IUNIT(16),
0219          1          IOUT)
0219          1          IOUT)
0220          IF (IUNIT(17).GT.0) CALL RES1AL (ISUM,LENX,LCIRES,LCIRSL,LCBRES,
0221          1          LCCRES,LCBBRE,LCHRES,LCHRSE,IUNIT(17),IOUT,NRES,IRESCB,
0222          2          NRESOP,IRESPT,NPTS,NCOL,NROW)
0223          C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>>
0224          c          IF (IUNIT(18).GT.0) CALL STR1AL (ISUM,LENX,LCSTRM,ICSTRM,MXSTRM,
0225          c          1          NSTREM,IUNIT(18),IOUT,ISTCB1,ISTCB2,NSS,NTRIB,
0226          c          2          NDIV,ICALC,CONST,LCTBAR,LCTTRIB,LCIVAR,LCFGAR)
0227          IF (IUNIT(18).GT.0) CALL STR1AL (ISUM,LENX,LCSTRM,ICSTRM,MXSTRM,
0228          1          NSTREM,IUNIT(18),IOUT,ISTCB1,ISTCB2,NSS,NTRIB,
0229          2          NDIV,ICALC,CONST,LCTBAR,LCTTRIB,LCIVAR,LCFGAR,
0230          3          iswabs,lctba2)
0231          C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0232          IF (IUNIT(19).GT.0) CALL IBS1AL (ISUM,LENX,LCHC,LCSCV,
0233          1          IBS)
0233          1          IBS)

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WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)

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0233      1      LCSUB,NCOL,NROW,NLAY,IIBSCB,IIBSOC,ISS,IUNIT(19),IOUT) IBS
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0234      IF(IUNIT(20).GT.0) CALL CHD1AL(ISUM,LENX,LCCHDS,NCHDS,MXCHD,      CHD      AT 0EB9
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0235      1      IUNIT(20),IOUT)      CHD
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0236      IF(IUNIT(21).GT.0) CALL FHB1AL(ISUM,LENX,LCFLLC,LCBDTM,LCFLRT,      AT 0EFD
0237      1      LCBDFV,LCBDHV,LCHDLC,LCSBHD,NBDTIM,NFLW,NHED,IUNIT(21),
0238      2      IOUT,IFHBCB,NFHBX1,NFHBX2,IFHBD3,IFHBD4,IFHBD5,
0239      3      IFHBSS,ISS)
0240      C
0241      C5-----IF THE "X" ARRAY IS NOT BIG ENOUGH THEN STOP.
0242      IF(ISUM-1.GT.LENX) STOP      AT 0FAA
0243      C
0244      C6-----READ AND PREPARE INFORMATION FOR ENTIRE SIMULATION.
0245      CALL BAS5RP(X(LCIBOU),X(LCHNEW),X(LCSTRT),X(LCHOLD),      AT 0FDO
0246      1      ISTRT,INBAS,HEADNG,NCOL,NROW,NLAY,VBVL,X(LCIOFL),
0247      2      IUNIT(12),IHEDFM,IDDNFM,IHEDUN,IDDNUM,IOUT,IPERO,ITSOC,
0248      3      CHEDFM,CDDNFM,IBDOPT,IXSEC,LBHDSV,LBDDSV,IFREFM)
0249      C-Environment Agency (UK)-0.General change to enable new options>>>>>>>>
0250      c      IF(IUNIT(1).GT.0) CALL BCF5RP(X(LCIBOU),X(LCHNEW),X(LCSC1),
0251      c      1      X(LCHY),X(LCCR),X(LCCC),X(LCCV),X(LCDELRL),
0252      c      2      X(LCDELRL),X(LCBOT),X(LCTOP),X(LCSC2),X(LCTRPY),IUNIT(1),
0253      c      3      ISS,NCOL,NROW,NLAY,IOUT,X(LCWETD),IWDFLG,X(LCCVWD))
0254      C-Environment Agency (UK)-16.K gradient independant of kbase>>>>>>>>>
0255      c      IF(IUNIT(1).GT.0) CALL BCF5RP(X(LCIBOU),X(LCHNEW),X(LCSC1),
0256      c      1      X(LCHY),X(LCCR),X(LCCC),X(LCCV),X(LCDELRL),
0257      c      2      X(LCDELRL),X(LCBOT),X(LCTOP),X(LCSC2),X(LCTRPY),IUNIT(1),
0258      c      3      ISS,NCOL,NROW,NLAY,IOUT,X(LCWETD),IWDFLG,X(LCCVWD),itryp,
0259      c      4      x(lckgrad),x(lcmid),x(lckmax),x(lcsgrad),x(lcsmax),x(lcsmid))
0260      IF(IUNIT(1).GT.0) CALL BCF5RP(X(LCIBOU),X(LCHNEW),X(LCSC1),      AT 10CA
0261      1      X(LCHY),X(LCCR),X(LCCC),X(LCCV),X(LCDELRL),
0262      2      X(LCDELRL),X(LCBOT),X(LCTOP),X(LCSC2),X(LCTRPY),IUNIT(1),
0263      3      ISS,NCOL,NROW,NLAY,IOUT,X(LCWETD),IWDFLG,X(LCCVWD),itryp,
0264      4      x(lckgrad),x(lcmid),x(lckmax),x(lcsgrad),x(lcsmax),x(lcsmid),
0265      5      ikbase)
0266      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0267      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0268      IF(IUNIT(6).GT.0) CALL TLK1RP(X(LCRAT),X(LCZCB),X(LCA1),X(LCB1),      AT 1244
0269      1      X(LCALPH),X(LCBET),X(LCRM1),X(LCRM2),X(LCRM3),X(LCRM4),
0270      2      NODES1,NM1,NM2,NUMC,NTM1,ITLKRS,DELTM1,X(LCBUFF),
0271      3      X(LCDELRL),X(LCDELRL),TLKTIM,NROW,NCOL,IUNIT(6),IOUT)
0272      IF(IUNIT(9).GT.0) CALL SIP5RP(NPARM,MXITER,ACCL,HCLOSE,X(LCW),      AT 1363
0273      1      IUNIT(9),IPCALC,IPRSIP,IOUT,IFREFM)
0274      IF(IUNIT(10).GT.0) CALL DE45RP(IUNIT(10),MXITER,NITER,ITMX,      AT 13C5
0275      1      ACCL,HCLOSE,IFREQ,IPRD4,IOUT,MUTD4)
0276      IF(IUNIT(11).GT.0) CALL SOR5RP(MXITER,ACCL,HCLOSE,IUNIT(11),      AT 1420
0277      1      IPRSOR,IOUT,IFREFM)
0278      IF(IUNIT(13).GT.0) CALL PCG2RP(MXITER,ITER1,HCLOSE,RCLOSE,      AT 1466
0279      1      NPCOND,NBPOL,RELAX,IPRPG,IUNIT(13),IOUT,MUTPCG,
0280      2      NITER,X(LCIT1),DAMP)
0281      IF(IUNIT(14).GT.0) CALL GFD1RP(X(LCIBOU),X(LCHNEW),X(LCSC1),      AT 14E4
0282      1      X(LCCDTR),X(LCCDTC),X(LCCR),X(LCCC),X(LCCV),X(LCDELRL),
0283      2      X(LCDELRL),X(LCBOT),X(LCTOP),X(LCSC2),
0284      3      IUNIT(14),ISS,NCOL,NROW,NLAY,NODES,IOUT)
0285      IF(IUNIT(16).GT.0) CALL HFBI1RP(X(LCCR),X(LCCC),X(LCDELRL),      *HFB* AT 15E0
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0286      1      X(LCDELRL),X(LCHFBR),IUNIT(16),NCOL,NROW,NLAY,NODES,      *HFB*
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0287      1      NHFB,IOUT)      *HFB*
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0288      IF(IUNIT(19).GT.0) CALL IBS1RP(X(LCDELRL),X(LCDELRL),X(LCHNEW),      IBS      AT 166C
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0289      1      X(LCHC),X(LCSCE),X(LCSCV),X(LCSUB),NCOL,NROW,NLAY,      IBS
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0290      2      NODES,IIBSOC,ISUBFM,ICOMFM,IHCFM,ISUBUN,ICOMUN,IHCUN,      IBS
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0291      3      IUNIT(19),IOUT)      IBS
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0292      IF(IUNIT(21).GT.0) CALL FHB1RP(X(LCIBOU),NROW,NCOL,NLAY,      AT 173E
0293      &      X(LCFLLC),X(LCBDTM),NBDTIM,X(LCFLRT),NFLW,NHED,
0294      &      X(LCHDLC),X(LCSBHD),IUNIT(21),IOUT,
0295      &      NFHBX1,NFHBX2,IFHBD3,IFHBD5)
0296      C
0297      C-Environment Agency (UK)-10.Convergence info output to screen>>>>>>>>
0298      IF(IUNIT(13).GT.0)then      AT 17FB
0299.01      write(*,5)' +-----+-----+-----+-----+-----+-----+
0300.01      endif      AT 1808
0301.01      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0302.01      C      AT 1848
0303.01      C7-----SIMULATE EACH STRESS PERIOD.
0304      DO 300 KPER=1,NPER      AT 1848

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0379.03          KKITER=KITER                                     AT 22AF
0380.03          C
0381.03          C7C2A---FORMULATE THE FINITE DIFFERENCE EQUATIONS.
0382.03          CALL BAS5FM(X(LCHCOF),X(LCRHS),NODES)           AT 22B5
0383.03          C-Environment Agency (UK)-0.General change to enable new options>>>>>>>>
0384.03          c      IF(IUNIT(1).GT.0) CALL BCF5FM(X(LCHCOF),X(LCRHS),X(LCHOLD)),
0385.03          c      1          X(LCSC1),X(LCHNEW),X(LCIBOU),X(LCCR),X(LCCC),X(LCCV),
0386.03          c      2          X(LCHY),X(LCTRPY),X(LCBOT),X(LCTOP),X(LCSC2),
0387.03          c      3          X(LCDELR),X(LCDELC),DELT,ISS,KKITER,KKSTP,KKPER,NCOL,
0388.03          c      4          NROW,NLAY,IOUT,X(LCWETD),IWDPLG,X(LCCVWD),WETFCT,
0389.03          c      5          IWETIT,IHDWET,HDRY,X(LCBUFF))
0390.03          IF(IUNIT(1).GT.0) CALL BCF5FM(X(LCHCOF),X(LCRHS),X(LCHOLD)),           AT 22E0
0391.03          1          X(LCSC1),X(LCHNEW),X(LCIBOU),X(LCCR),X(LCCC),X(LCCV),
0392.03          2          X(LCHY),X(LCTRPY),X(LCBOT),X(LCTOP),X(LCSC2),
0393.03          3          X(LCDELR),X(LCDELC),DELT,ISS,KKITER,KKSTP,KKPER,NCOL,
0394.03          4          NROW,NLAY,IOUT,X(LCWETD),IWDPLG,X(LCCVWD),WETFCT,
0395.03          5          IWETIT,IHDWET,HDRY,X(LCBUFF),itrpy,x(lckgrad),ihold,
0396.03          6          x(lcmid),x(lckmax),x(lcsgrad),x(lcsmax),x(lcsmid)
0397.03          C-Environment Agency (UK)-End of this section of modified code <<<<<<<<<
0398.03          IF(IUNIT(14).GT.0) CALL GFD1FM(X(LCHCOF),X(LCRHS),X(LCHOLD)),           AT 24C6
0399.03          1          X(LCSC1),X(LCHNEW),X(LCIBOU),X(LCCR),X(LCCC),X(LCCV),
0400.03          2          X(LCCDTR),X(LCCDTC),X(LCBOT),X(LCTOP),X(LCSC2),
0401.03          3          DELT,ISS,KKITER,KKSTP,KKPER,NCOL,NROW,NLAY,IOUT)
0402.03          IF(IUNIT(16).GT.0) CALL HFB1FM(X(LCHNEW),X(LCCR),X(LCCC),           *HFB* AT 25DE
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0403.03          1          X(LCBOT),X(LCTOP),X(LCDELR),X(LCDELC),X(LCHFBR),           *HFB*
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0404.03          2          NCOL,NROW,NLAY,NHFB)           *HFB*
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0405.03          IF(IUNIT(6).GT.0) CALL TLK1FM(X(LCRAT),X(LCTL),X(LCTLK),X(LCSLU)),           AT 267F
0406.03          1          X(LCSLD),NUMC,X(LCHNEW),X(LCIBOU),X(LCTOP),X(LCCV),
0407.03          2          X(LCHCOF),X(LCRHS),NROW,NCOL,NLAY)
0408.03          IF(IUNIT(2).GT.0) CALL WEL5FM(NWELLS,MXWELL,X(LCRHS),X(LCWELL)),           AT 274A
0409.03          1          X(LCIBOU),NCOL,NROW,NLAY,NWELVL)
0410.03          IF(IUNIT(3).GT.0) CALL DRN5FM(NDRAIN,MXDRN,X(LCDRAI),X(LCHNEW)),           AT 27B3
0411.03          1          X(LCHCOF),X(LCRHS),X(LCIBOU),NCOL,NROW,NLAY,NDRNVL)
0412.03          IF(IUNIT(4).GT.0) CALL RIV5FM(NRIVER,MXRIVR,X(LCRIVR),X(LCHNEW)),           AT 2838
0413.03          1          X(LCHCOF),X(LCRHS),X(LCIBOU),NCOL,NROW,NLAY,NRIVVL)
0414.03          IF(IUNIT(5).GT.0) CALL EVT5FM(NEVTOP,X(LCIEVT),X(LCEVTR),           AT 28BD
0415.03          1          X(LCEXDP),X(LCSURF),X(LCRHS),X(LCHCOF),X(LCIBOU),
0416.03          1          X(LCHNEW),NCOL,NROW,NLAY)
0417.03          IF(IUNIT(7).GT.0) CALL GHB5FM(NBOUND,MXBND,X(LCBNDS),X(LCHCOF)),           AT 295E
0418.03          1          X(LCRHS),X(LCIBOU),NCOL,NROW,NLAY,NGBVVL)
0419.03          IF(IUNIT(8).GT.0) CALL RCH5FM(NRCHOP,X(LCIRCH),X(LCRECH)),           AT 29D5
0420.03          1          X(LCRHS),X(LCIBOU),NCOL,NROW,NLAY)
0421.03          IF(IUNIT(17).GT.0) CALL RES1FM(X(LCIRSL),X(LCIRSL),X(LCBRES)),           AT 2A3E
0422.03          1          X(LCCRES),X(LCBBRE),X(LCHRES),X(LCIBOU),X(LCHNEW),X(LCHCOF),
0423.03          2          X(LCRHS),NRES,NRESOP,NCOL,NROW,NLAY)
0424.03          C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>>
0425.03          c      IF(IUNIT(18).GT.0) CALL STR1FM(NSTREM,X(LCSTRM),X(ICSTRM),           STR1
0426.03          c      1          X(LCHNEW),X(LCHCOF),X(LCRHS),X(LCIBOU),           STR1
0427.03          c      2          MXSTRM,NCOL,NROW,NLAY,IOUT,NSS,X(LCTBAR),           STR1
0428.03          c      3          NTRIB,X(LCTRIB),X(LCIVAR),X(LCFGAR),ICALC,CONST)           STR1
0429.03          IF(IUNIT(18).GT.0) CALL STR1FM(NSTREM,X(LCSTRM),X(ICSTRM)),           STR1 AT 2B02
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0430.03          1          X(LCHNEW),X(LCHCOF),X(LCRHS),X(LCIBOU),           STR1
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0431.03          2          MXSTRM,NCOL,NROW,NLAY,IOUT,NSS,X(LCTBAR),           STR1
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0432.03          3          NTRIB,X(LCTRIB),X(LCIVAR),X(LCFGAR),ICALC,CONST,           STR1
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0433.03          4          iswabs,x(lctba2))           STR1
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0434.03          C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0435.03          IF(IUNIT(19).GT.0) CALL IBS1FM(X(LCRHS),X(LCHCOF),X(LCHNEW)),           IBS AT 2BFE
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0436.03          1          X(LCHOLD),X(LCHC),X(LCSCE),X(LCSCV),X(LCIBOU),           IBS
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0437.03          2          NCOL,NROW,NLAY,DELT)           IBS
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0438.03          IF(IUNIT(21).GT.0) CALL FHB1FM(X(LCRHS),X(LCIBOU),X(LCFLLC)),           AT 2C9F
0439.03          1          X(LCBDFV),NFLW,NCOL,NROW,NLAY,IFHBD4)
0440.03          C
0441.03          C7C2B---MAKE ONE CUT AT AN APPROXIMATE SOLUTION.
0442.03          IF(IUNIT(9).GT.0) CALL SIP5AP(X(LCHNEW),X(LCIBOU),X(LCCR),X(LCCC)),           AT 2D0F
0443.03          1          X(LCCV),X(LCHCOF),X(LCRHS),X(LCEL),X(LCFL),X(LCGL),X(LCV),
0444.03          2          X(LCW),X(LCHDCG),X(LCLRCH),NPARM,KKITER,HCLOSE,ACCL,ICNVG,
0445.03          3          KKSTP,KKPER,IPCALC,IPRSIP,MXITER,NSTP,NCOL,NROW,NLAY,NODES,
0446.03          4          IOUT)
0447.03          IF(IUNIT(10).GT.0) CALL DE45AP(X(LCHNEW),X(LCIBOU),X(LCAU)),           AT 2E58
0448.03          1          X(LCAL),X(LCIUPP),X(LCIEQP),X(LCD4B),MXUP,MXLOW,MXBQ,MXBW,
0449.03          2          X(LCCR),X(LCCC),X(LCCV),X(LCHCOF),X(LCRHS),ACCL,KKITER,ITMX,

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0450.03      3  MXITER,NITER,HCLOSE,IPRD4,ICNVG,NCOL,NROW,NLAY,IOUT,X(LCLRCH),
0451.03      4  X(LCHDCG),IFREQ,KKSTP,KKPER,DELT,NSTP,ID4DIR,ID4DIM,MUTD4)
0452.03      IF(IUNIT(11).GT.0) CALL SORSAP(X(LCHNEW),X(LCIBOU),X(LCCR),
AT 2FDC
0453.03      1  X(LCCC),X(LCCV),X(LCHCOF),X(LCRHS),X(LCA),X(LCRES),X(LCIEQP),
0454.03      2  X(LCHDCG),X(LCLRCH),KKITER,HCLOSE,ACCL,ICNVG,KKSTP,KKPER,
0455.03      3  IPRSOR,MXITER,NSTP,NCOL,NROW,NLAY,NSLICE,MBW,IOUT)
0456.03      C-Environment Agency (UK)-0.General change to enable new options>>>>>>>
0457.03      c  IF(IUNIT(13).GT.0) CALL PCG2AP(X(LCHNEW),X(LCIBOU),X(LCCR),
0458.03      c  1  X(LCCC),X(LCCV),X(LCHCOF),X(LCRHS),X(LCV),X(LCSS),X(LCP),
0459.03      c  2  X(LCCD),X(LCHCHG),X(LCLHCH),X(LCRCHG),X(LCLRCH),KKITER,
0460.03      c  3  NITER,HCLOSE,RCLOSE,ICNVG,KKSTP,KKPER,IPRPGC,MXITER,ITER1,
0461.03      c  4  NPCOND,NBPOL,NSTP,NCOL,NROW,NLAY,NODES,RELAX,IOUT,MUTPCG,
0462.03      c  5  0,0,SN,SP,SR,X(LCIT1),DAMP)
0463.03      IF(IUNIT(13).GT.0) CALL PCG2AP(X(LCHNEW),X(LCIBOU),X(LCCR),
AT 3102
0464.03      1  X(LCCC),X(LCCV),X(LCHCOF),X(LCRHS),X(LCV),X(LCSS),X(LCP),
0465.03      2  X(LCCD),X(LCHCHG),X(LCLHCH),X(LCRCHG),X(LCLRCH),KKITER,
0466.03      3  NITER,HCLOSE,RCLOSE,ICNVG,KKSTP,KKPER,IPRPGC,MXITER,ITER1,
0467.03      4  NPCOND,NBPOL,NSTP,NCOL,NROW,NLAY,NODES,RELAX,IOUT,MUTPCG,
0468.03      5  0,0,SN,SP,SR,X(LCIT1),DAMP,noutc,nout,ipcgdebug,ixsec,
0469.03      6  chedfm,x(lcbuf),lbhdsv)
0470.03      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0471.03      C
0472.03      C-Environment Agency (UK)-10.Convergence info output to screen>>>>>>>>
0473.03      IF(IUNIT(13).GT.0.and.NITER.gt.0)then
AT 32EA
0474.04      write(*,501)KKPER,KKSTP,NITER,X(LCHCHG+NITER-1),
AT 3304
0475.04      1  X(LCRCHG+NITER-1)
0476.04      endif
AT 33B6
0477.03      501 format(' |',i7,' |',i5,' |',i6,' |',g11.4,' |',g11.4,' |')
AT 33B6
0478.03      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0479.03      C
0480.03      C7C2C---IF CONVERGENCE CRITERION HAS BEEN MET STOP ITERATING.
0481.03      IF(ICNVG.EQ.1) GO TO 110
AT 340B
0482.03      100 CONTINUE
AT 3418
0483.02      KITER=MXITER
AT 341D
0484.02      110 CONTINUE
AT 3429
0485.02      C
0486.02      C7C3---DETERMINE WHICH OUTPUT IS NEEDED.
0487.02      CALL BAS5OC(NSTP,KKSTP,ICNVG,X(LCIOFL),NLAY,IBUDFL,ICBCFL,
AT 3429
0488.02      1  IHDDFL,IUNIT(12),IOUT,KKPER,IPERO,ITSOC,IBDOPT,IXSEC,IFREFM)
0489.02      C
0490.02      C7C4---CALCULATE BUDGET TERMS. SAVE CELL-BY-CELL FLOW TERMS.
0491.02      MSUM=1
AT 34A8
0492.02      IF(IUNIT(6).GT.0) CALL TLK1BD(X(LCRAT),X(LCTL),X(LCTLK),
AT 34B2
0493.02      1  X(LCSLU),X(LCSLD),NUMC,ITLKCB,X(LCHNEW),X(LCIBOU),X(LCIBUFF),
0494.02      2  X(LCIBOU),X(LCTOP),X(LCCV),VBNM,VBVL,MSUM,NCOL,NROW,
0495.02      3  NLAY,DELT,KSTP,KPER,ICBCFL,IOUT)
0496.02      C7C4A---THE ORIGINAL BCF BUDGET MODULE HAS BEEN REPLACED BY THREE
0497.02      C7C4A---SUBMODULES: SBCF5S, SBCF5F, AND SBCF5B .
0498.02      IF(IUNIT(1).GT.0) THEN
AT 35B4
0499.02      C-Environment Agency (UK)-2.Variable storage with depth (VSD)>>>>>>>>
0500.02      c  CALL SBCF5S(VBNM,VBVL,MSUM,X(LCHNEW),X(LCIBOU),X(LCHOLD),
0501.02      c  1  X(LCSC1),X(LCTOP),X(LCSC2),DELT,ISS,NCOL,NROW,NLAY,KKSTP,
0502.02      c  2  KKPER,IBCFB,ICBCFL,X(LCIBUFF),IOUT,PERTIM,TOTIM)
0503.03      CALL SBCF5S(VBNM,VBVL,MSUM,X(LCHNEW),X(LCIBOU),X(LCHOLD),
AT 35C1
0504.03      1  X(LCSC1),X(LCTOP),X(LCSC2),DELT,ISS,NCOL,NROW,NLAY,KKSTP,
0505.03      2  KKPER,IBCFB,ICBCFL,X(LCIBUFF),IOUT,PERTIM,TOTIM,x(lcbot),
0506.03      3  x(lcmid),x(lcsgrad),x(lcsmax),x(lcsmid)
0507.03      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0508.03      CALL SBCF5F(VBNM,VBVL,MSUM,X(LCHNEW),X(LCIBOU),X(LCCR),
AT 36E0
0509.03      1  X(LCCC),X(LCCV),X(LCTOP),DELT,NCOL,NROW,NLAY,KKSTP,KKPER,
0510.03      2  IBCFCB,X(LCIBUFF),IOUT,ICBCFL,PERTIM,TOTIM,ICHFLG)
0511.03      IBDRET=0
AT 37B9
0512.03      IC1=1
AT 37C3
0513.03      IC2=NCOL
AT 37CD
0514.03      IR1=1
AT 37D9
0515.03      IR2=NROW
AT 37E3
0516.03      IL1=1
AT 37EF
0517.03      IL2=NLAY
AT 37F9
0518.03      DO 155 IDIR=1,3
AT 3805
0519.04      CALL SBCF5B(X(LCHNEW),X(LCIBOU),X(LCCR),X(LCCC),X(LCCV),
AT 3822
0520.04      1  X(LCTOP),NCOL,NROW,NLAY,KKSTP,KKPER,IBCFB,X(LCIBUFF),
0521.04      2  IOUT,ICBCFL,DELT,PERTIM,TOTIM,IDIR,IBDRET,ICHFLG,
0522.04      3  IC1,IC2,IR1,IR2,IL1,IL2)
0523.04      155 CONTINUE
AT 3918
0524.03      END IF
AT 391D
0525.02      IF(IUNIT(14).GT.0) CALL GFD1BD(VBNM,VBVL,MSUM,X(LCHNEW),
AT 391D
0526.02      1  X(LCIBOU),X(LCHOLD),X(LCSC1),X(LCCR),X(LCCC),X(LCCV),
0527.02      2  X(LCTOP),X(LCSC2),DELT,ISS,NCOL,NROW,NLAY,KKSTP,KKPER,
0528.02      3  IGFDCB,ICBCFL,X(LCIBUFF),IOUT)
0529.02      IF(IUNIT(2).GT.0) CALL WEL5BD(NWELLS,MXWELL,VBNM,VBVL,MSUM,
AT 3A1F
0530.02      1  X(LCWELL),X(LCIBOU),DELT,NCOL,NROW,NLAY,KKSTP,KKPER,IWELCB,
0531.02      1  ICBCFL,X(LCIBUFF),IOUT,PERTIM,TOTIM,NWELVL,IWELAL)

```

```

0532.02      IF (IUNIT(3).GT.0) CALL DRN5BD (NDRAIN, MXDRN, VBNM, VBVL, MSUM,
0533.02      1      X (LCDRAI), DELT, X (LCHNEW), NCOL, NROW, NLAY, X (LCIBOU), KKSTP,
0534.02      2      KKPER, IDRNCB, ICBCFL, X (LCBUFF), IOUT, PERTIM, TOTIM, NDRNVL,
0535.02      3      IDRNAL)
0536.02      IF (IUNIT(4).GT.0) CALL RIV5BD (NRIVER, MXRIVR, X (LCRIVR), X (LCIBOU),
0537.02      1      X (LCHNEW), NCOL, NROW, NLAY, DELT, VBVL, VBNM, MSUM, KKSTP, KKPER,
0538.02      2      IRIVCB, ICBCFL, X (LCBUFF), IOUT, PERTIM, TOTIM, NRIVVL, IRIVAL)
0539.02      IF (IUNIT(5).GT.0) CALL EVT5BD (NEVTOP, X (LCIEVT), X (LCEVTR),
0540.02      1      X (LCEXDP), X (LCSURF), X (LCIBOU), X (LCHNEW), NCOL, NROW, NLAY,
0541.02      2      DELT, VBVL, VBNM, MSUM, KKSTP, KKPER, IEVTCB, ICBCFL, X (LCBUFF), IOUT,
0542.02      3      PERTIM, TOTIM)
0543.02      IF (IUNIT(7).GT.0) CALL GHB5BD (NBOUND, MXBND, VBNM, VBVL, MSUM,
0544.02      1      X (LCBND), DELT, X (LCHNEW), NCOL, NROW, NLAY, X (LCIBOU), KKSTP,
0545.02      2      KKPER, IGHBCB, ICBCFL, X (LCBUFF), IOUT, PERTIM, TOTIM, NGHVBVL,
0546.02      3      IGHBAL)
0547.02      IF (IUNIT(8).GT.0) CALL RCH5BD (NRCHOP, X (LCIRCH), X (LCRECH),
0548.02      1      X (LCIBOU), NROW, NCOL, NLAY, DELT, VBVL, VBNM, MSUM, KKSTP, KKPER,
0549.02      2      IRCHCB, ICBCFL, X (LCBUFF), IOUT, PERTIM, TOTIM)
0550.02      IF (IUNIT(17).GT.0) CALL RES1BD (X (LCIRES), X (LCIRSL), X (LCBRES),
0551.02      1      X (LCCRES), X (LCBBRE), X (LCHRES), X (LCIBOU), X (LCHNEW),
0552.02      2      X (LCBUFF), VBVL, VBNM, MSUM, KSTP, KPER, NRES, NRESOP,
0553.02      3      NCOL, NROW, NLAY, DELT, IRESCB, ICBCFL, IOUT)
0554.02      C-Environment Agency (UK)-14.Allow in/outflow or trib at any reach>>>>>
0555.02      c      IF (IUNIT(18).GT.0) CALL STR1BD (NSTREM, X (LCSTRM), X (ICSTRM), STR1
0556.02      c      1      X (LCIBOU), MXSTRM, X (LCHNEW), NCOL, NROW, NLAY, DELT, VBVL, VBNM, MSUM, STR1
0557.02      c      2      KKSTP, KKPER, ISTCB1, ISTCB2, ICBCFL, X (LCBUFF), IOUT, NTRIB, NSS, STR1
0558.02      c      3      X (LCTTRIB), X (LCTBAR), X (LCIVAR), X (LCFGAR), ICALC, CONST, IPTFLG) STR1
0559.02      IF (IUNIT(18).GT.0) CALL STR1BD (NSTREM, X (LCSTRM), X (ICSTRM), STR1 AT 3FF2
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0560.02      1      X (LCIBOU), MXSTRM, X (LCHNEW), NCOL, NROW, NLAY, DELT, VBVL, VBNM, MSUM, STR1
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0561.02      2      KKSTP, KKPER, ISTCB1, ISTCB2, ICBCFL, X (LCBUFF), IOUT, NTRIB, NSS, STR1
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0562.02      3      X (LCTTRIB), X (LCTBAR), X (LCIVAR), X (LCFGAR), ICALC, CONST, IPTFLG, STR1
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0563.02      4      iswabs,x(lctba2)) STR1
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0564.02      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0565.02      IF (IUNIT(19).GT.0) CALL IBS1BD (X (LCIBOU), X (LCHNEW), X (LCHOLD), IBS AT 412F
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0566.02      1      X (LCHC), X (LCSCE), X (LCSCV), X (LCSUB), X (LCDEL), X (LCDEL), IBS
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0567.02      2      NCOL, NROW, NLAY, DELT, VBVL, VBNM, MSUM, KSTP, KPER, IIBSCB, IBS
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0568.02      3      ICBCFL, X (LCBUFF), IOUT) IBS
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0569.02      IF (IUNIT(21).GT.0) CALL FHB1BD (X (LCFLLC), X (LCBDFV), NFWLW,
0570.02      1      VBNM, VBVL, MSUM, X (LCIBOU), DELT, NCOL, NROW, NLAY, KKSTP, KKPER,
0571.02      2      IFHBCB, ICBCFL, X (LCBUFF), IOUT, IFHBD4)
0572.02      C
0573.02      C-Environment Agency (UK)-8.Output calculated transmissivities>>>>>>>>>>>>
0574.02      C7C4B--PRINT INTERNODAL TRANSMISSIVITIES IF ITRANS IS NOT ZERO
0575.02      C-Environment Agency (UK)-17.Output calc trans to binary file>>>>>>>>>>>>
0576.02      c      if (itrans.ne.0) call bcf5ot (x (lccc), x (lccr), x (lcbuff), kkstp,
0577.02      c      1      kkper, ncol, nrow, nlay, iout, ixsec, x (lccdelc), x (lccdelr), itrpy,
0578.02      c      2      x (lctrpy), ihedfm, x (lccv))
0579.02      if (itrans.ne.0) call bcf5ot (x (lccc), x (lccr), x (lcbuff), kkstp, AT 42DF
0580.02      1      kkper, ncol, nrow, nlay, iout, ixsec, x (lccdelc), x (lccdelr), itrpy,
0581.02      2      x (lctrpy), ihedfm, x (lccv), itrans, X (LCIOFL), CHEDFM, LBHDSV,
0582.02      3      X (LCIBOU), PERTIM, TOTIM)
0583.02      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0584.02      C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0585.02      c
0586.02      C7C5---PRINT AND OR SAVE HEADS AND DRAWDOWNS. PRINT OVERALL BUDGET.
0587.02      CALL BAS5OT (X (LCHNEW), X (LCSTRT), ISTRT, X (LCBUFF), X (LCIOFL), AT 43DA
0588.02      1      MSUM, X (LCIBOU), VBNM, VBVL, KKSTP, KKPER, DELT, PERTIM, TOTIM,
0589.02      2      ITMUNI, NCOL, NROW, NLAY, ICNVG, IHDDFL, IBUDFL, IHEDFM, IHEDUN,
0590.02      3      IDDNFM, IDDNUN, IOUT, CHEDFM, CDDNFM, IXSEC, LBHDSV, LBDDSV)
0591.02      C
0592.02      C7C5A--PRINT AND OR SAVE SUBSIDENCE, COMPACTION, AND CRITICAL HEAD.
0593.02      IF (IUNIT(19).GT.0) CALL IBS1OT (NCOL, NROW, NLAY, PERTIM, TOTIM, KSTP, IBS AT 44F3
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0594.02      1      KPER, NSTP, X (LCBUFF), X (LCSUB), X (LCHC), IIBSOC, ISUBFM, ICOMFM, IBS
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0595.02      2      IHCNM, ISUBUN, ICOMUN, IHCUN, IUNIT(19), IOUT) IBS
WARNING - Characters found after column 72 (use -NO_WARN73 to suppress)
0596.02      C
0597.02      C7C6----IF ITERATION FAILED TO CONVERGE THEN STOP.
0598.02      C-Environment Agency (UK)-10.Convergence info output to screen>>>>>>>>>>>>
0599.02      c      IF (ICNVG.EQ.0) STOP
0600.02      IF (ICNVG.EQ.0) then AT 45A9
0601.03      write(*,*) AT 45B6

```



```

0602.03         write(*,*) ' *** Failed to converge ***'                AT 45D2
0603.03         STOP                                                    AT 4606
0604.03         endif                                                    AT 4619
0605.02         IF(IUNIT(13).GT.0)then                                    AT 4619
0606.03         write(*,5) ' +-----+-----+-----+-----+-----+' AT 4626
0607.03         endif                                                    AT 4666
0608.03 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0609.03 C
0610.02         200 CONTINUE                                             AT 4666
0611.01         300 CONTINUE                                             AT 466B
0612.01 C
0613.01 C7C7---WRITE RESTART RECORDS
0614.01 C7C7A---WRITE RESTART RECORDS FOR TRANSIENT-LEAKAGE PACKAGE
0615         IF(IUNIT(6).GT.0) CALL TLK1OT(X(LCRM1),X(LCRM2),            AT 4670
0616         1         X(LCRM3),X(LCRM4),NM1,NM2,ITLKSV,DELTM1,TLKTIM,IOUT)
0617
0618 C-Environment Agency (UK)-3.Auto-conversion for steady state VKD>>>>>>>>
0619 C7D-----IF USING AUTOMATIC CONVERSION OPTION, CLOSE ALL CONNECTED FILES,
0620 C7D----- (EXCEPT THE MAIN OUTPUT FILE), CALL ROUTINE TO WRITE NEW INPUT
0621 C7D-----FILES AND RETURN TO THE START OF THE PROGRAM TO RUN THE SECOND
0622 C7D-----PART OF THE SIMULATION WITH VKD ACTIVE.
0623         if(iss.eq.2.or.iss.eq.3)then                                  AT 46E7
0624.01         do 355 i=1,ibouts-1
0625.02             inquire(unit=i,opened=exists)                        AT 472D
0626.02             inquire(unit=i,named=exists2)                        AT 474F
0627.02             if(exists.and.exists2)then                            AT 4774
0628.03                 if(i.ne.iout)close(i)                            AT 478B
0629.03             endif                                                AT 47B6
0630.02         355 continue                                             AT 47B6
0631.01         call BCF5VK(x(lchnew),inunit,iunit(1),inbas,ibcfoutunit, AT 47BB
0632.01         1             inoutunit,ioutbas,ncol,nrow,nlay,ifrefm,fname,cunit(1),
0633.01         2             IXSEC,NPER,iout,x(lcIBOU),x(lcHOLD),x(lcTRPY),x(lcDELR),
0634.01         3             x(lcDELC),x(lcSC1),x(lcCC),x(lcHY),x(lcBOT),x(lcCV),
0635.01         4             x(lcTOP),x(lcSC2),x(lckgrad),x(lcWETD),x(lcbuff),x(lccr),
0636.01         5             x(lcmid),x(lckmax))
0637.01         do 350 i=1,ibouts-1                                        AT 4936
0638.02             inquire(unit=i,opened=exists)                        AT 4962
0639.02             inquire(unit=i,named=exists2)                        AT 4984
0640.02             if(exists.and.exists2)then                            AT 49A9
0641.03                 close(i)                                          AT 49C0
0642.03             endif                                                AT 49D9
0643.02         350 continue                                             AT 49D9
0644.01         go to 55
0645.01         end if                                                    AT 49DE
0646.01 C-Environment Agency (UK)-End of this section of modified code <<<<<<<<
0647.01 C
0648.01 C8-----END OF SIMULATION
0649         IF(IBATCH.GT.0) THEN                                        AT 49E3
0650.01             WRITE(IBOUTS,*) ' Normal termination of simulation.' AT 49ED
0651.01             DO 400 I=1,IBOUTS-1
0652.02                 INQUIRE(UNIT=I,OPENED=EXISTS)                    AT 4A20
0653.02                 IF(EXISTS) CLOSE(I)                                AT 4A4C
0654.02         400 CONTINUE                                             AT 4A6E
0655.01             GO TO 50                                              AT 4A91
0656.01         END IF                                                    AT 4A93
0657         500 STOP                                                    AT 4A98
0658 C
0659         END                                                            AT 4AAB

```

End of compilation - Clocked 0.0 seconds

APPENDIX F
Further testing of the MODFLOW VKD code

FURTHER TESTING OF THE MODFLOW VKD CODE

ENVIRONMENT AGENCY

**NATIONAL GROUNDWATER &
CONTAMINATED LAND CENTRE**

**FURTHER TESTING OF THE
MODFLOW VKD CODE**

September 2003

1821/R2

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APPENDICES

A	Results of the test problems
B	Contents of the CD included in the revised version of the User Guide for MODFLOW-VKD

1 INTRODUCTION

1.1 Background

This report describes the work undertaken by Water Management Consultants (WMC) following a request received from the Environment Agency (EA), National Groundwater and Contaminated Land Centre (NGWCLC) for further testing of MODFLOW-VKD.

MODFLOW-VKD was developed, documented and tested by WMC under the NGWCLC Project NC/00/23. The code of MODFLOW-VKD includes modifications that allow the simulation of variable hydraulic conductivity and storage with depth within a model layer. The code and User Guide for MODFLOW-VKD (EA, 2002a and EA, 2003) were provided by WMC to the NGWCLC initially in April 2002.

The work described in this report implements the contents of the proposal detailed in the letter *Further testing of the MODFLOW VKD Code, Groundwater Technical Services Contract #11589*, which was submitted to the NGWCLC on 30 October 2002.

This report was prepared as an appendix to be inserted in the September 2003 revised version of the MODFLOW-VKD User Guide, initially published in March 2002 (EA, 2002). For the Agency Sarah Evers was Project Manager and Paul Hulme the Project Board.

1.2 Objectives

The main objective of the work is to ascertain that the modifications introduced to produce variable hydraulic conductivity (K) and storage (S) with depth have not altered the core function of MODFLOW. This involves examining whether the results produced by the VKD version of the code used for simulations with no requirement for variable K and S with depth are the same as those generated by the unaltered MODFLOW. Additional objectives include checking whether the use of different compilers to create the executable for MODFLOW-VKD affects the model output and defining how MODFLOW-VKD can be used in conjunction with the particle-tracking program, MODPATH (USGS, 1994) and the optimisation and sensitivity analysis program, UCODE (USGS, 1998).

1.3 Structure of report

Section 2 presents the methodology that was employed to compare the results produced by the unmodified and VKD version of MODFLOW. Section 3 describes the execution of the test problems and details the implications of using MODFLOW-VKD in combination with MODPATH (USGS, 1994) and UCODE (USGS, 1998), whilst Section 4 contains a summary, conclusions and recommendations related to the further testing of MODFLOW-VKD. Appendix A includes the tables describing each test problem.

2 METHODOLOGY

The VKD version of MODFLOW enables the simulation of variable hydraulic conductivity and storage with depth within a model layer. A series of tests are performed to verify that the VKD modifications have not altered the basic function of MODFLOW.

The following tests were employed:

- 12 of the 20 US EPA instructional problems available with associated documentation at <http://www.epa.gov/ada/csmos/models/modflow.html>. These tests were developed to give users experience in the use of MODFLOW and provide a documented testing of the code.
- 7 problems available at the USGS web site where MODFLOW 96 can be downloaded, <http://water.usgs.gov/software/modflow-96.html>. Documentation for 4 of these tests is available at the same web site. These tests are designed to illustrate and test specific boundary conditions such as the lake and inter-bed storage packages.
- The Wirral groundwater model. This is a relatively large time-variant model of the Permo-Triassic Sandstone developed by the EA North-West Region with assistance from WMC (EA, 2002).
- The GPZ model for the Tadcaster brewery boreholes. The model was developed and documented by WMC for the EA North-East Region (EA, 1997). This test is employed to run MODPATH (USGS, 1994) in combination with MODFLOW-VKD.
- A variation on one of the original test models used for testing MODFLOW-VKD (EA, 2002). This test is employed to run the USGS optimisation and sensitivity analysis program, UCODE (USGS, 1998), in combination with MODFLOW-VKD.

The tests are based on a model that was run using the following versions of MODFLOW:

- unmodified MODFLOW-96 code (MF96), obtained from <http://water.usgs.gov/software/modflow-96.html> and compiled with the Salford FORTRAN77 compiler to produce the executable MODFLW96.exe.
- MODFLOW-VKD (MF-VKD), compiled with the Salford 77 compiler to produce the executable MF-VKD1.exe¹. This executable was provided by Water Management Consultants to the EA, NGWCLC in April 2002. The MF-VKD1.exe executable was the first release of the VKD code. Subsequently, further development has continued such that at the time of writing the current VKD executable is MF-VKD7.exe
- The executables of MF96 and MF-VKD compiled with the Compaq FORTRAN77 compiler. These were employed on two tests (problem 1 and 2 of the USGS suite) in order to verify whether the use of a different compiler would generate differences in the results produced by the two model versions.

For each test, the following model runs were performed:

- A. Use of MF96.
- B. Use of MF-VKD with the VKD function inactive. This means that no data required to account for a variation of K and S with depth were introduced. The input dataset was modified only by removing the comments on the first line of the .BCF file, in order to make its input format compatible with MF-VKD.
- C. Use of MF-VKD with the VKD function active. This means that data required to account for a variation of K and S with depth were introduced. In order to make the comparison between the results of this run and those generated by MF96 meaningful, the VKD parameters were set so that the hydraulic properties of the test model would not alter.

In addition to the above runs, further simulations were performed on some of the test problems, as follows:

- C1. Problems 1 and 2 in the USGS suite. Use of MF-VKD (with the VKD function active) compiled using the Compaq FORTRAN compiler, which is available to the Environment Agency.
- D. GPZ Tadcaster model. Use of the auto-conversion option available within MF-VKD to produce a depth-dependent K field, which reproduces the transmissivity associated with the model steady-state solution.

The pre-conjugate gradient (PCG2) solver is not employed in most of the test models in the US EPA and USGS suite, despite being the most efficient in the execution of real, complex models. For this reason, an additional run based on the use of the PCG2 package was performed on Test Problem 8 and 12 (problems 13 and 20 of the EPA series). Note that the Environment Agency discourages the use of the SOR and SIP matrix solvers for MODFLOW due to potential inaccuracies in solutions as discussed in Osiensky and Williams (1997).

Three types of modifications to the test model dataset were applied:

- Modifications aimed at producing output files that would contain sufficient information on flows and heads to allow a thorough comparison between the results produced by the unmodified and VKD version of MODFLOW. These modifications are detailed in Section 2.1.
- Modifications aimed at making the format of the input dataset compatible with MF-VKD. These consisted only in removing the comments in the first line of the .BCF file when they were placed in positions employed in MF-VKD to define some VKD parameters.
- Modifications aimed at reproducing the hydraulic properties of the test model using VKD parameters. The means of reproducing the hydraulic properties of a model using VKD parameters is detailed in Section 2.2.

2.1 Set-up and comparison of output

The test model datasets were modified in order to generate the output files with the following extensions:

- OUT file with heads, drawdowns and volumetric budgets printed at the end of each time step.
- CBB file with all flow components printed at the end of each time step.

In order to produce these output files the input dataset was modified as follows:

- NAM file:

Replace the first line with

```
LIST 6 *_new_X.OUT
```

Replace the last line with

```
DATA (BINARY) 50 *_new_X.CBB
```

The symbol * represents the root name for the test model and X is the run type (A, B, C, C1, D).

- BAS file:

Set ISTRT = 1 (flag to save starting heads, so that drawdowns can be calculated).

- OC file:

For each time step, set IHDDFL = 1, ICBCFL = 1, IBUDFL = 1 (save or print heads and drawdowns, cell-by-cell flow and volumetric budget). Set INCODE = 0 (read output head/ddn specifications on one line and apply to all model layers), Hdpr = 1 and Ddpr = 1 (print or save heads and drawdowns) in the first time step, INCODE = -1 (apply same output head/ddn specifications as in previous time step) in the following time steps.

- BCF and other flow component files (e.g. .WEL, .DRN):

Set I*CB = 50 (unit where flow component is saved), where * represents the extension of the flow component file (e.g. IWELCB, IDRNCB).

Detailed instructions on how to specify the output settings in the MODFLOW files are provided in the MODFLOW Manual (USGS, 1996).

The output files were compared according to the following procedure:

- OUT files.

These are ASCII files that can be viewed in any text editor. Ultra Edit-32©, version 6.20b was used (IDM Computer Solutions, 1999), since it can open large files and has a 'Compare files...' facility that creates a text file listing the lines where the files exhibit differences. The comparison files were named comp_out_*_XY.txt, where * represents the root name of the model dataset and X and Y are the runs (A, B, C, C1, D) being compared.

- CBB files.

These are binary files that cannot be directly viewed with a text editor. An ASCII version of these files was created using the utility program cbc2gv.exe developed by WMC, which was given the same root name as the .CBB file and a .DAT extension. The ASCII files were then compared using the 'Compare files...' facility within Ultra Edit-32. The comparison files were named comp_cbb_*_XY.txt, where * represents the root name of the model dataset and X and Y are the runs (A, B, C, C1, D) being compared.

The .CBB files produced in the two tests where MF-VKD1 is compiled by the Compaq FORTRAN compiler are in a different binary format from those generated by MF-VKD compiled by the Salford FORTRAN compiler. As a consequence, they cannot be recognised by cbc2gv.exe, which operates on .CBB files in the binary format produced with MF compiled using the Salford compiler. In order to create the ASCII version of the .CBB files, these were therefore produced as direct access binary files. This was achieved by modifying the last line of the name file as follows:

```
from          DATA (BINARY) 50  *_new_X.CBB
to            DATA (BINARY) 50  *_new_gvX.CBB DIRECT 1.
```

The ASCII version of these .CBB files was then created using the utility cbc2dos.exe, which reads direct access binary files.

2.2 Set-up of VKD function

In order to activate the VKD function in run C of each test as described in Section 2, the following parameters need to be assigned:

- LAYCON (4 for unconfined conditions, 5 for confined-unconfined conditions)
- For each model layer:
 - If the simulation is in time-variant mode
 - Sf1 (**Sbase**, base unconfined storage coefficient)
 - HY (**Kbase**, base hydraulic conductivity)
 - **BOT** (layer bottom elevation)
 - If not the bottom layer
 - VCONT
 - If LAYCON = 5 and the simulation is in time-variant mode
 - Sf2 (confined storage coefficient)
 - If LAYCON = 5
 - **TOP** (layer top elevation)
 - If the wetting capability is active
 - WETDRY (combination of wetting threshold and flag indicating which neighboring cells can cause a cell to become wet)
 - **VMID** (elevation of the point of inflection for hydraulic conductivity, where hydraulic conductivity changes from being constant to varying with depth)
 - **VKGRAD** (gradient factor applied to the zone where hydraulic conductivity is variable. It is multiplied by the base hydraulic conductivity to give the hydraulic conductivity gradient)
 - **VKMAX** (the maximum hydraulic conductivity factor applied to the zone where hydraulic conductivity is variable. It is multiplied by the base hydraulic conductivity to give the maximum hydraulic conductivity)

- If the simulation is in time-variant mode
 - **VSMID** (elevation of the point of inflection for the unconfined storage coefficient, where the unconfined storage coefficient changes from being constant to varying with depth)
 - **VSGRAD** (unconfined storage coefficient gradient factor applied to the zone where the unconfined storage coefficient is variable. It is multiplied by the base unconfined storage coefficient to give the unconfined storage coefficient gradient)
 - **VSMAX** (the maximum unconfined storage coefficient factor applied to the zone where the unconfined storage coefficient is variable. It is multiplied by the base unconfined storage coefficient to give the maximum unconfined storage coefficient).

The VKD parameters in bold are represented in Figures 1a and 1b, which show the conceptual model for the variation of hydraulic conductivity and storage coefficient with depth as illustrated in the MF-VKD User Guide, Figures 2.1 and 2.2 (EA, 2003).

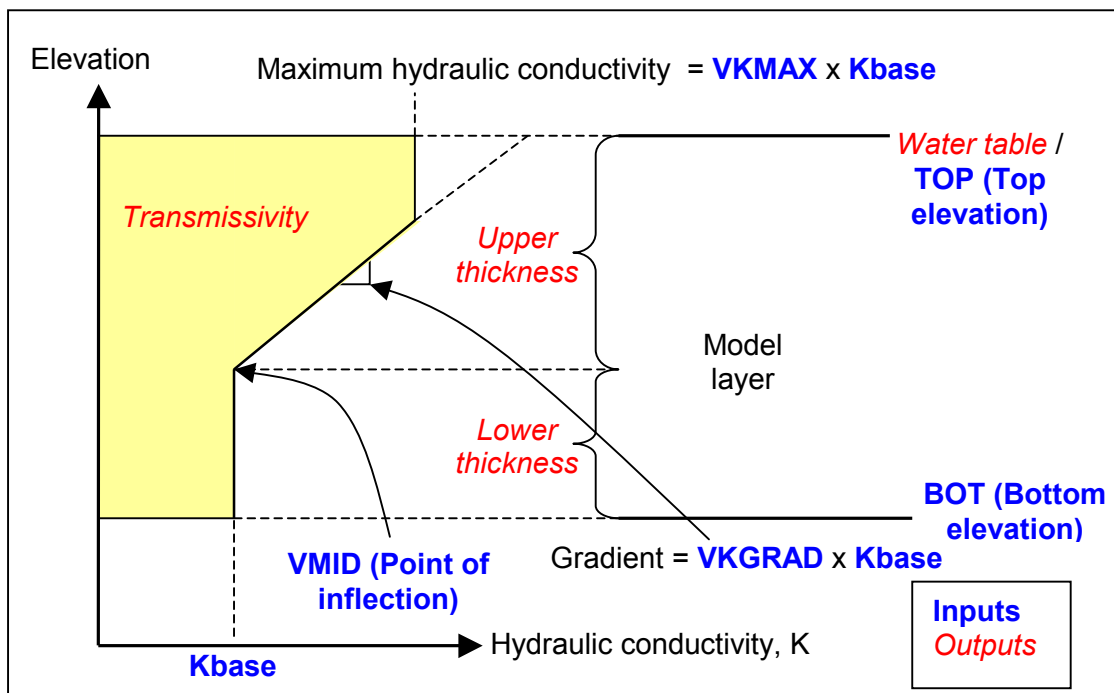


Figure 1a Conceptual model for the variation of hydraulic conductivity with depth

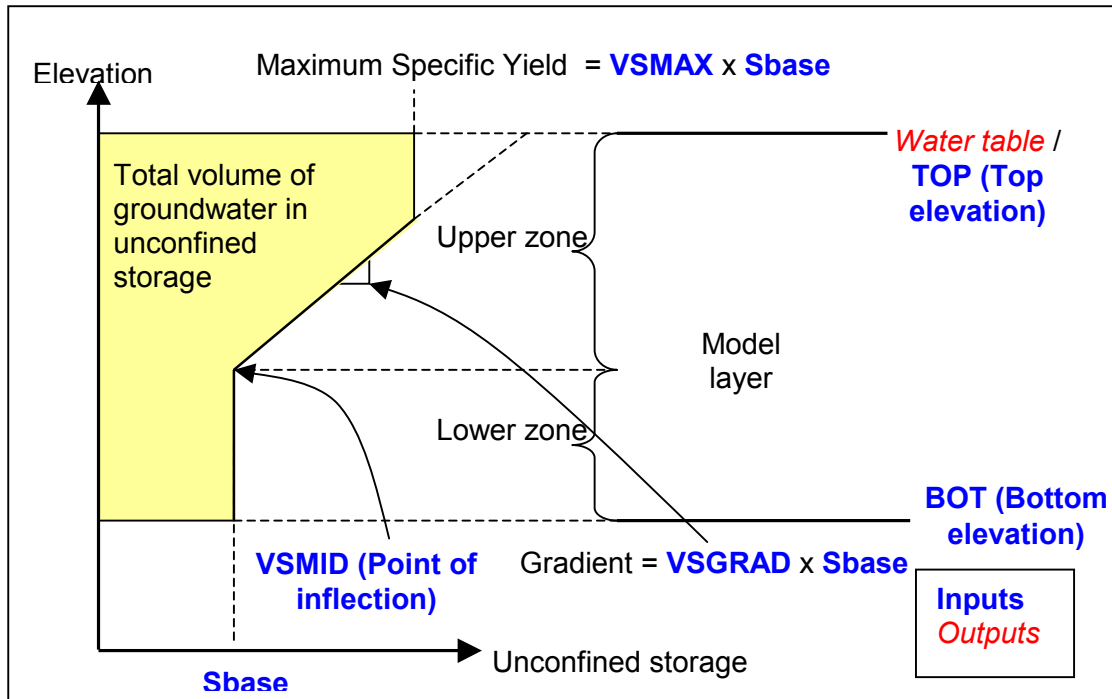


Figure 1b Conceptual model for the variation of storage with depth

The listed VKD parameters are assigned in the .BCF file according to the format described in the MF-VKD User Guide (EA, 2003).

In order to reproduce the hydraulic properties of the test models using the VKD parameters, the following settings have been applied:

- LAYCON value conversion. For the VKD function to be active, a value of 4 (unconfined conditions) or 5 (confined-unconfined conditions) must be assigned to LAYCON. Table 1 shows the conversion between the LAYCON value according to the unmodified MODFLOW and the VKD LAYCON value with associated comments.

Table 1 Conversion of LAYCON values from MF96 to MF-VKD

LAYCON according to unmodified MODFLOW	VKD LAYCON	Comments
0	5	Strictly confined conditions. These can be reproduced by setting values of TOP and BOT that are guaranteed to be always lower than the head range throughout the simulation. The difference between TOP and BOT is set to 1, so that values of transmissivity, T, used by unmodified MODFLOW are equal to the values of the base hydraulic conductivity, Kbase, used by MODFLOW-VKD.
1	4	Unconfined conditions.
2	N/A	Confined-unconfined conditions where T is constant and S varies over time. It is not possible to reproduce these conditions with LAYCON = 5, as both T and S vary over time.
3	5	Confined-unconfined conditions where T and S vary over time.

- VMID (and VSMID values in time-variant simulations) is set equal to BOT. This means that the inflection point is placed at the bottom of the layer.
- VKGRAD (and VSGRAD in time-variant simulations) is set equal to 1. This means that a linear variation of K (S) of $1 \times K_{base}$ ($1 \times S_{base}$) occurs for a unit change in depth within the layer.
- VKMAX (and VSMAX values in time-variant simulations) is set equal to 1. This means that K (S) is kept equal to K_{base} (S_{base}) within the layer, thus overriding the variation set with VKGRAD (VSGRAD).

The VKD parameter setting described in the above three bullet points is shown in Figure 1c.

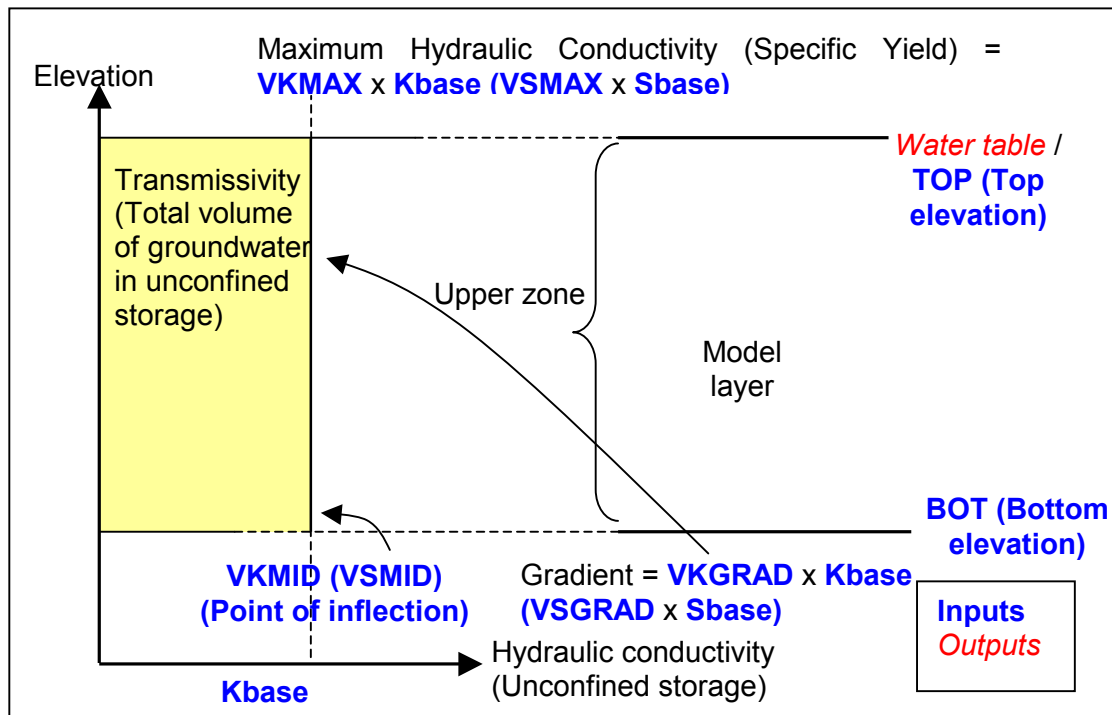


Figure 1c Representation of depth-uniform hydraulic conductivity (unconfined storage) using VKD parameters

3 EXECUTION OF TEST PROBLEMS

The test models employed to identify the differences between the results produced by the unmodified and VKD version of MODFLOW are detailed in the tables shown in Appendix A. For each test, the following information is provided:

- Model name and dataset root name.
- Reference documentation (USGS / US EPA / EA report where the model is described).
- Aim and brief description of test.
- Input files required in test.
- Changes required for execution with MF96 and MF-VKD (changes in output setting not included).
- Type of differences identified between the output files generated by MF96 and MF-VKD, with VKD function active and inactive.

The type of differences identified between the output files generated by the unmodified and VKD version of MODFLOW were classified as follows:

- Differences in headers and comments in the .OUT file. These are differences in the format of the output files that are not problem-specific, ie the same differences were identified in all tests. These differences are not related to a change in the basic MODFLOW functionality due to the presence of VKD components and are therefore not mentioned in the test summary tables.
- Differences in memory allocation printed in the .OUT file. The VKD version of MODFLOW increases the size of the X-array, a general array where MODFLOW stores most of its variable arrays, from 1,500,00 to 10,000,000 elements (an element being equal to 4 bytes). Different numbers of elements from the X-array are also allocated for the variable arrays required by the BCF and other packages employed in each test model. These differences do not compromise the basic MODFLOW functionality due to the presence of VKD components and are therefore not mentioned in the test summary tables.

- Differences in the values of head, drawdown, components of the volumetric budget of cell-by-cell flows in the .OUT and .DAT version of the .CBB file. “Type I” differences are defined as small differences in global flow between balance components (i.e. less than 0.1%), and in heads and drawdowns (less than 1%). These are due to round-off errors deriving from the use of different parameters and variables in the calculation of the coefficients of the flow equation in MF96 and MF-VKD. In particular, some of the parameters and variables employed by MF-VKD to calculate storage coefficients and conductances are declared in the source file BCF-VKD6.for (subroutines BCF5FM, SBCF5S, SBCF5H and bcf5vk) using double precision. Larger differences (defined as “Type II”) may be related to a change in the basic MODFLOW functionality due to the presence of VKD components and therefore need further investigation.

Whenever differences between the drawdowns, heads and maximum changes in heads during an iteration emerge in the .OUT files generated by the MF96 and MF-VKD (VKD function active and inactive), the associated cell-by cell flows are compared by subtraction within Excel, in order to identify whether significant discrepancies are present.

3.1 GPZ model testing

The unmodified and VKD version of MODFLOW were run in combination with MODPATH using the flow and particle-tracking model employed to define groundwater protection zones for the Tadcaster brewery boreholes. The model was developed for the Environment Agency, Northeast Region, by WMC (EA, 1997). The version of the model employed in the test is referred as Tad401. This model version was used to define the Outer and Total Catchment Zone for the source 0577 (EA, 1997). The MODPATH files for this model were created using the ‘Create dataset’ facility within GWVistas. MODPATH version 3.0 included in the GWVistas software was used to perform this test. In order to run MODPATH outside GWVistas, the MODPATH input files generated by GWVistas were renamed and modified as follows:

- Response file, mpath.rsp. This file was renamed mpath_Tad401.rsp and the name file listed in it was renamed.
- Name file, modpath.dat. This file was renamed mpath_Tad401.dat.
- The head and cell-by-cell flow file names were replaced by *Tad401_new_gvX.hds* and *Tad401_new_gvX.cbb*, respectively, where X indicates the run type (A, B, C, D). These are direct access binary files that are created from the binary files produced by MF96 and MF-VKD using the utilities hds2gv.exe and cbc2gv.exe. Direct access binary files are required by the version of MODPATH available within GWVistas. It is noted that direct access binary files can be created directly by MF96 and MF-VKD by adding the expression DIRECT 1 after the name of the head and cell-by-cell flow file listed in the .NAM file. The reason why this method was not employed to create the direct binary .CBB files required by MODPATH in this test is that the utilities hds2gv.exe and cbb2gv.exe were used to convert the .CBB files into direct access binary format as well into ASCII, .DAT format.
- The files *Tad401_X.ept* and *Tad401_X.ptl* are added to the file list. These files contain information about the particle final positions and the particle pathlines, respectively.

The results generated by the runs performed for this test were compared using the .OUT, the ASCII version of the .CBB and .HDS files.

Besides the runs A, B and C, an additional run, D, was performed in this test. The purpose of this run is to ascertain that the VKD function works correctly. In this run, hydraulic conductivity is set to vary with depth in such a way that the transmissivity resulting from integration over the steady-state saturated thickness produced by the unmodified MODFLOW is the same as the steady-state transmissivity based on the constant hydraulic conductivity field of the original model.

This is illustrated in Figure 2, where K_0 is the original hydraulic conductivity and the remaining parameters are the same as those shown in Figures 2.1 and 2.2 in the MF-VKD User Guide (EA, 2003).

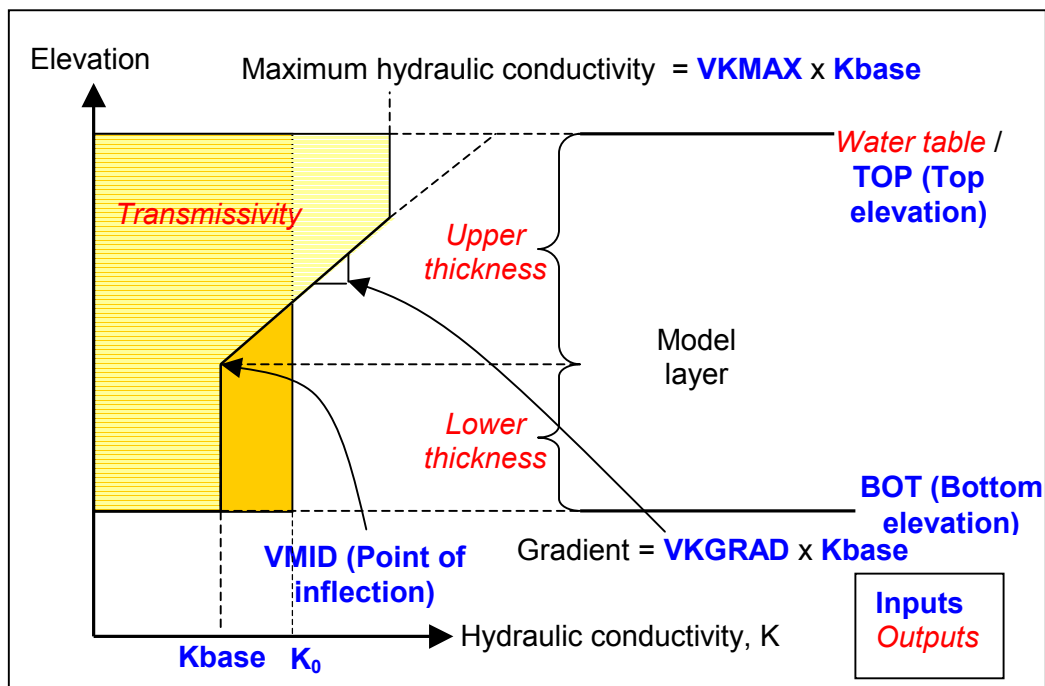


Figure 2 Equivalence between transmissivity associated with constant and depth-variable hydraulic conductivity

The auto-conversion option available in MF-VKD was employed to define the depth-dependent hydraulic conductivity field. The use of the auto-conversion option is described in Sections 3.3 and 8.4.1 of the MF-VKD User Guide (EA, 2003). The following VKD parameters were set in the .BCF file (renamed tad401auto.bcf) to define the hydraulic conductivity field:

- ISS (steady-state) flag = 3.
- ITRANS = 1 (flag specifying that internodal transmissivities will be output to the .OUT file).
- Thickness of upper zone = 5 m (this value is automatically re-set equal to the saturated thickness whenever the saturated thickness value is less than 5 m).
- VKGRAD = 1.
- VKMAX = 3.

Run D was performed using variable K with depth as described above and employing the steady-state heads produced by MF96 as initial conditions. Steady-state heads are used as initial conditions to ensure that the simulation converges on a solution quickly. The correct functioning of VKD is verified in this test by checking that the steady-state heads produced by MF-VKD are identical to the initial conditions, i.e. the steady-state heads generated by MF96. The differences in heads calculated by runs A and D were checked and found to be less than 0.02 m throughout the model domain.

The pathlines generated by MODPATH coupled with MF96, Run A, and MF-VKD, Run D, after 10000 days are shown in Figure 3a in three dimensions for the entire modelled domain, whereas Fig 3b zooms on two of the pathlines generated by the two model versions in order to highlight their discrepancy.

Figure 3b shows that the pathlines generated by MODPATH using the MF96 and MF-VKD head and cell-by-cell flow files have non-negligible discrepancies, with a maximum distance between pathlines of 113 m (in three dimensions). The comparison between the .ptl files produced by MODPATH based on the heads and flows generated by MF96 and MF-VKD in runs A and D confirms the presence of differences in the particle positions, travel times and number of cells that particles cross along their pathline.

The reason for the differences in the positions of the pathlines calculated by runs A and D is due to small differences between the heads and flows calculated by these runs. The maximum head difference between the two models should not exceed twice the head convergence criterion of 0.01 m. The difference of 0.017 falls within the expected range. Due to large values of hydraulic conductivity ($1000 \text{ m}^2/\text{d}$) and large contrasts in K from one cell to the next (of up to 100:1 at the main fissure locations), small head differences result in rather larger differences in flow. The maximum difference in flow is $15 \text{ m}^3/\text{d}$. This is less than twice the flow convergence criterion of $8 \text{ m}^3/\text{d}$.

The differences in head are due in part to the very slightly different values of transmissivity being used in simulations A and D. With VKD active very small rounding errors are introduced when calculating the base hydraulic conductivities in the auto-conversion simulation. This leads to the small differences in transmissivity values and consequently to slightly different calculations being used during the iterative process, resulting in a slightly different solution being found. Since the maximum differences are so slight, of the same order as the models convergence criteria, they do not in any way affect the validation of the VKD code. Whilst tighter convergence criteria would reduce head and flow differences, it was found that the large contrasts in hydraulic conductivity present in the model proved troublesome, and the model failed to converge.

The differences in head, and more particularly the differences in flow, affect the trajectory of the pathlines calculated by MODPATH. If the trajectories are changed enough that a flowline enters a different cell (in comparison to the previous simulation – this may be the result of only very small changes in trajectory), then the different flow conditions in that cell will have a greater influence in further diverting the trajectory of that flowline.

In the Tadcaster model runs A and D the maximum horizontal difference in pathline locations is around 30 m. The pathlines subsequently converge. The pathlines diverge at the locations of high contrast in hydraulic conductivity located around the fissures as described above. Around this area of the model the model cells have sides of 100 m. As the precision in the locations of the fissures is determined by the cell size, it can be seen that the uncertainty in the position of the pathline is less than a third of the uncertainty in the location of the fissure. It should also be noted that this 30 m discrepancy is small compared to the changes to pathline positions produced in sensitivity analysis (as used, for instance, in defining source protection zones).

So, whilst slight differences in pathlines have been found, they are due to very small rounding errors. The resulting head and flow discrepancies are dependant on the model convergence criteria and have no affect on the validity of the VKD code.

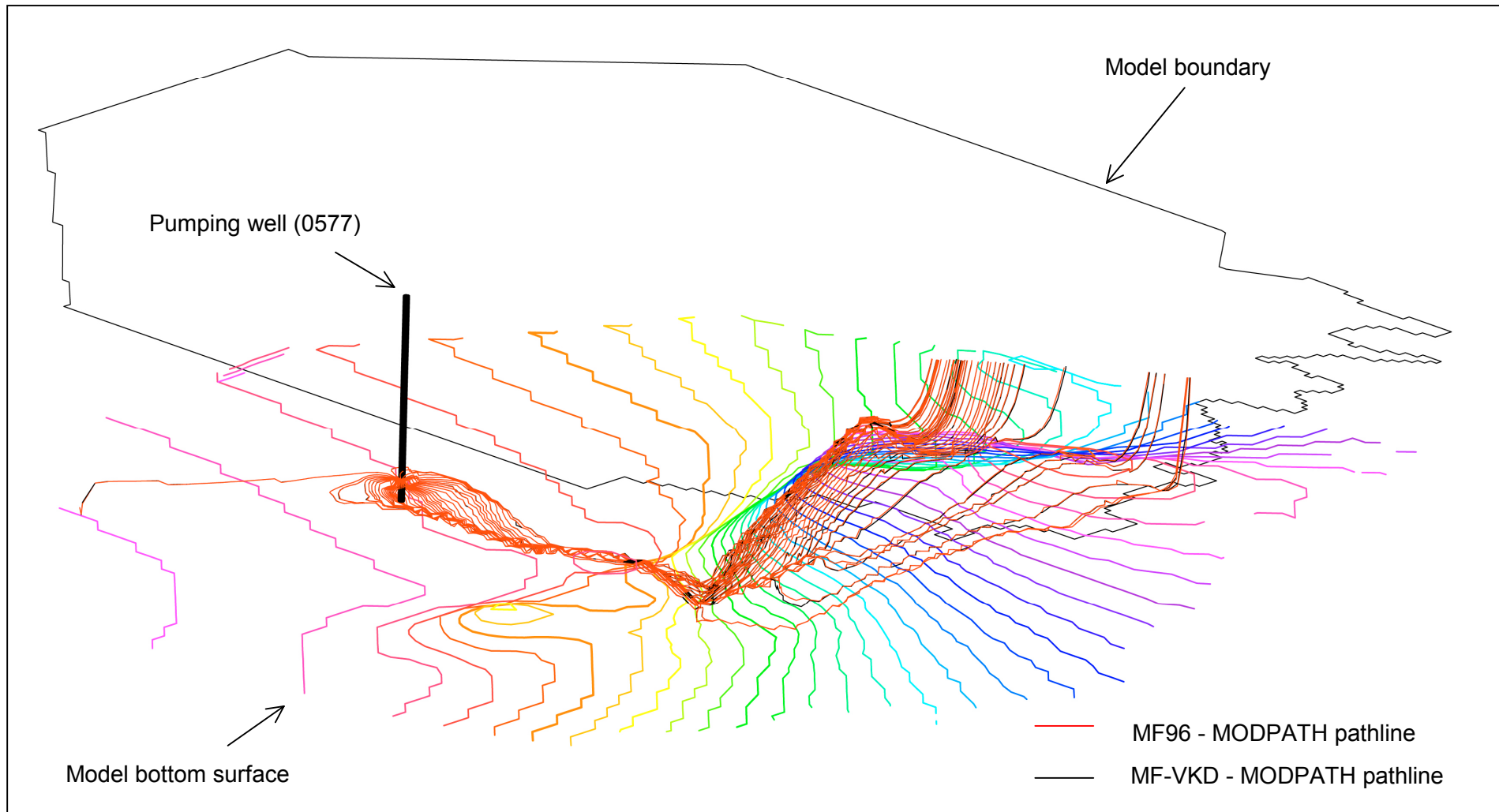


Figure 3a 3D view of pathlines generated by MF96 and by MF-VKD with depth-variable K yielding the same steady-state transmissivity – full model domain

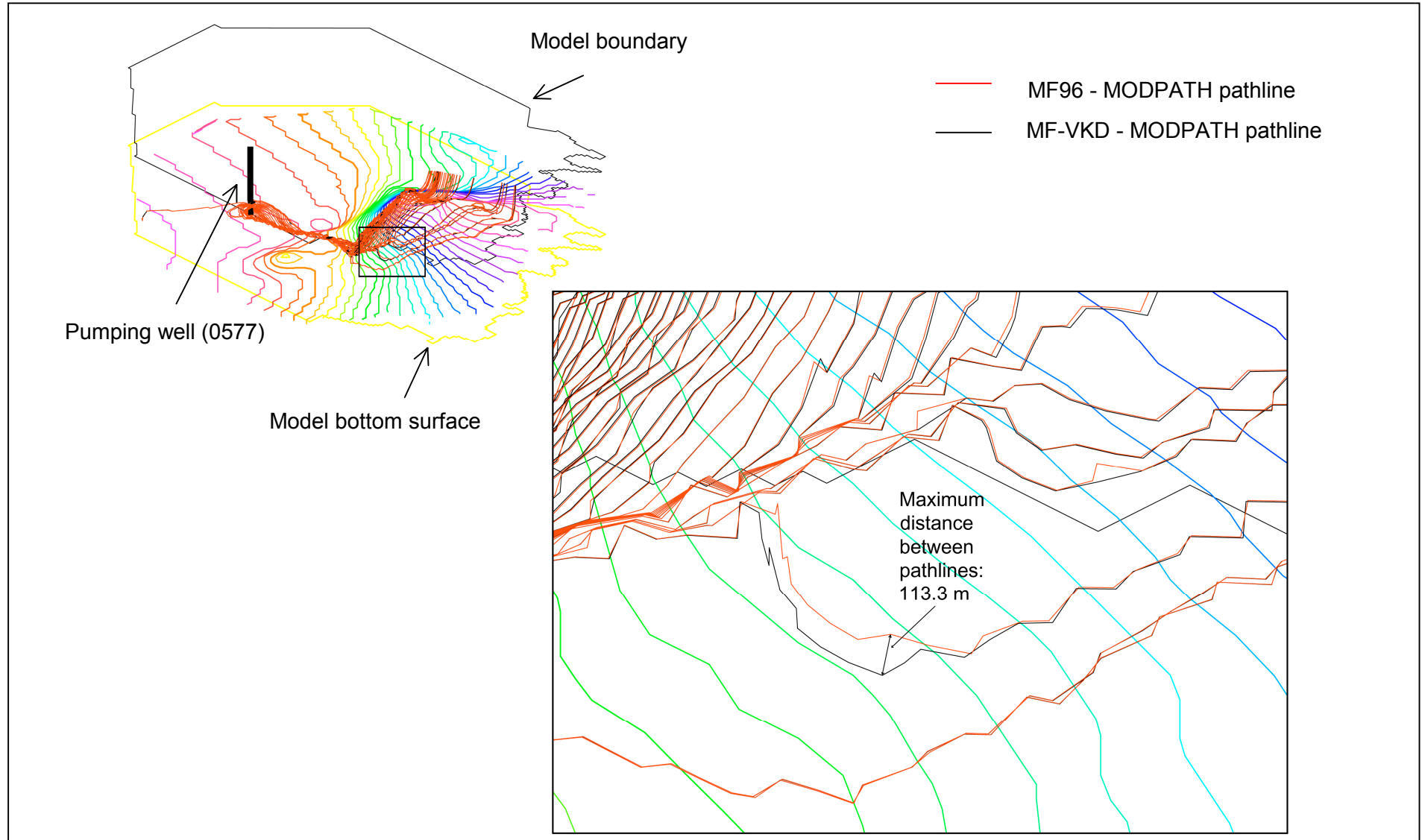


Figure 3b Example of discrepancy between the pathlines generated by MF96 and by MF-VKD with depth-variable K yielding the same steady-state transmissivity

3.2 Implications of performing particle tracking with VKD

When running MODPATH using the results of a model where VKD is used to set variable hydraulic conductivity with depth within a layer, attention must be drawn to how MODPATH computes the velocities used to define particle pathlines. In MODPATH average velocities across the faces of each cell are computed and are assumed to be constant within the cell face. These velocities are calculated by dividing the volume flow rates across the cell faces by the cell cross sectional areas and the cell porosity. The velocity of a particle located within a cell is then calculated by means of linear interpolation of the velocities defined at the cell faces.

The use of constant, depth-averaged velocities for each cell face means that MODPATH does not account correctly for the variation of hydraulic conductivity with depth within a model layer.

The implication of how MODPATH computes velocities is that when particle tracking is performed on a flow model where VKD is present, velocities can be under or over-estimated, according to the depth at which particles are released. In particular, the velocities for particles released in the low K zone will be over-estimated, whereas velocities for particles released in the high K zone will be under-estimated.

When particle tracking is applied with VKD to identify groundwater protection zones (GPZs) as in the Tadcaster model, run D, described in Section 3.1, the under-estimation of velocities for particles moving in the high K zone equates to the definition of smaller zones. Figure 4 compares particle tracks to a well for a standard MODPATH simulation to those that would be expected if MODPATH took VKD into account.

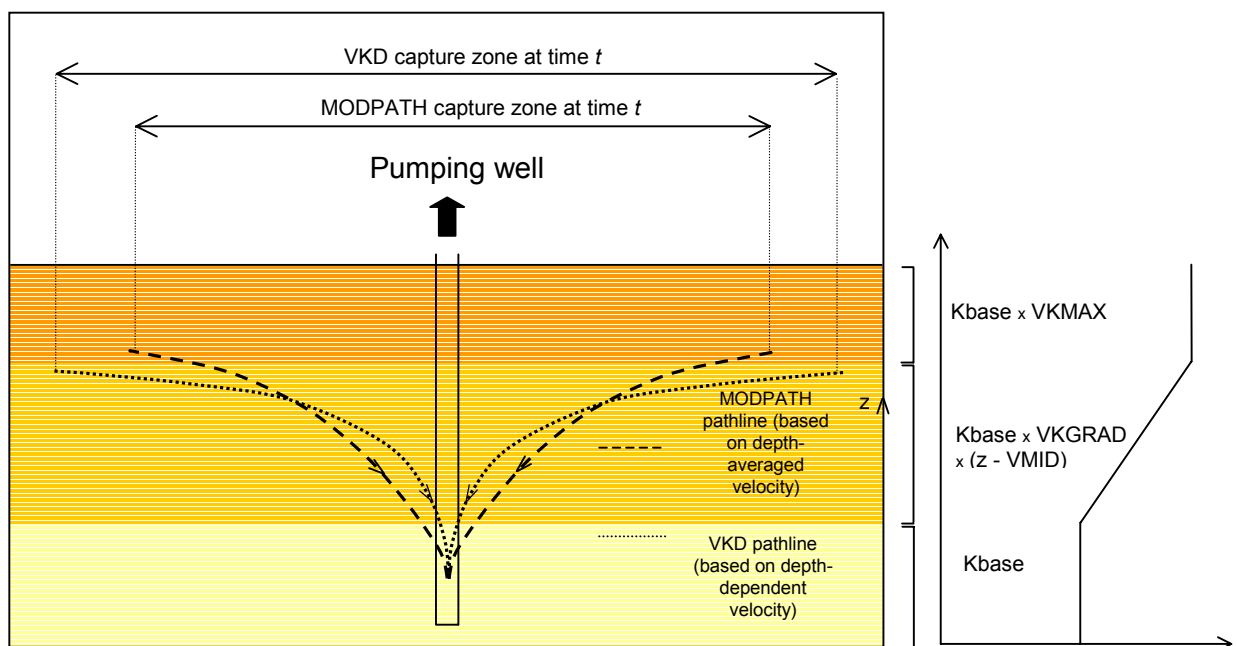


Figure 4 Effect of velocity computation method on pathlines

In order to reproduce fully the effect of variable K with depth, velocities across the faces of a cell should be computed in MODPATH as the ratio between the Darcy velocity and porosity, ie

$$v_i(z) = \frac{1}{\phi} \frac{k(z)\Delta h}{\Delta x_i}$$

where

$v_i(z)$: velocity in i direction at elevation z within the cell face

$k(z)$: hydraulic conductivity at elevation z

Δh : head difference across the cell face

Δx_i : distance between the centres of the cells separated by the cell face

ϕ : porosity

Using the above expression, velocities would no longer be constant but would vary with depth within a cell face according to K, and pathlines would be calculated accordingly.

3.3 Execution of test using UCODE

UCODE is a sensitivity analysis and parameter estimation program developed by the USGS (USGS, 1998). In order to explore if MODFLOW-VKD can be made to work with UCODE, one of the test models used in the original testing program was applied. The aim of this test was to use UCODE to calculate the sensitivity of VKD parameters.

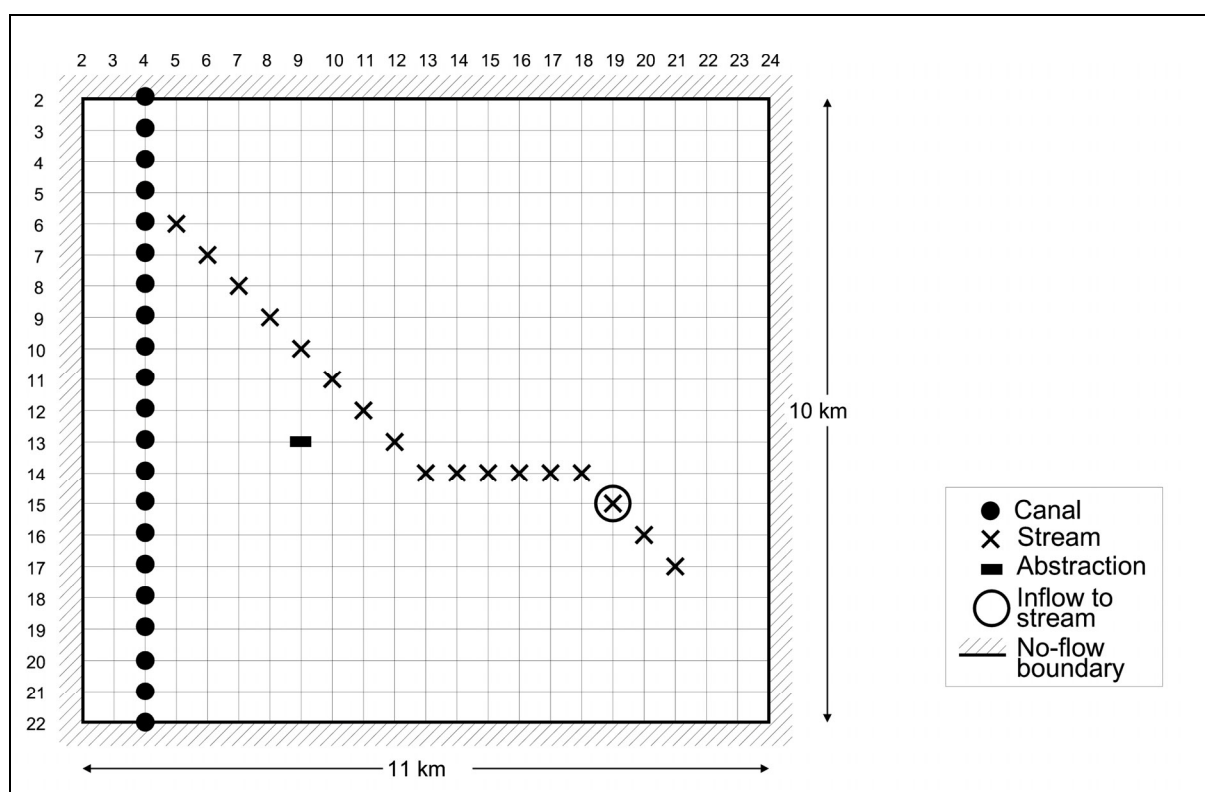


Figure 5 Simple model used for UCODE testing

Simple modifications were necessary to the VKD dataset with more detailed changes to UCODE input files. The testing model is a simple time-variant model of a hypothetical aquifer system with VKD, inflows from areal recharge and discharges to a well, a river and a stream (Figure 5). The model is described in more detail in the Enhancements to MODFLOW VKD report (EA, 2002a).

The model was run using MODFLOW-VKD in conjunction with UCODE. The following modifications were made to the MODFLOW input files:

- The name (*.nam) file was changed so that the binary files were written in direct access format (by adding 'DIRECT 1' after the relevant file names). This was done so that the Groundwater Vistas program 'targpest' could be used to extract simulated head values. These could then be used by UCODE to evaluate the sensitivity of the VKD parameters.
- The Block Centred Flow (BCF) package was modified so that the value for the hydraulic conductivity gradient factor (VKGRAD) was replaced by the label '!VKGRAD1,!'. The file was then saved as a template file, which would then be used by UCODE to create the .BCF file, the label being replaced by different values to evaluate the sensitivity of this parameter.

The UCODE input files were then created as follows:

- The universal input file (*.uni) was set up to do a sensitivity simulation (PHASE=2) and contained details of the batch file required to run MODFLOW-VKD and 'targpest'. It also contained details of dummy observed values at a point in the centre of the model, varying over time.
- The prepare file (*.pre) gave details of the filenames of the template and .BCF files, along with details relating to the parameter to be varied, VKGRAD.
- The extract file (*.ext) gave instructions to UCODE on how to extract the simulated head values from the output file created by 'targpest'.
- A file called 'targpest.dat' was created to allow 'targpest' to extract head values from the MODFLOW heads file (*.hds) to the output file, 'targpest.out'.
- An application model batch file containing the commands to run MODFLOW-VKD ('mf-vkd1 <mfvkd.in') and 'targpest'.
- The input file ('mfvkd.in') containing the filename of the MODFLOW name file (*.nam).
- The UCODE batch file containing the command required to run UCODE ('perl ucode ucode1 0')

By looking at the main output file produced by UCODE, ucode1._ot, it was checked that UCODE ran successfully, executing MODFLOW-VKD and 'targpest' three times to evaluate the sensitivity of the simulated heads to changes in the hydraulic conductivity gradient factor. It is concluded that UCODE can be successfully applied to MF-VKD models once necessary alterations are made to data files.

4 SUMMARY, CONCLUSIONS AND RECOMMENDATIONS

This section summarises the results of the testing, draws conclusions about whether the VKD code modifications have changed the basic function of MODFLOW and makes some limited recommendations concerning the use of MF-VKD. Full results of each test problem are presented in Appendix A.

4.1 Summary of results

A series of tests were performed using the MF-96 and MF-VKD versions of MODFLOW to ensure that the VKD modifications do not affect the basic function of MODFLOW. The tests include:

- A suite of instructional models developed by the US EPA.
- Examples illustrating specific MODFLOW packages developed by the USGS.
- A resource assessment model for the Wirral peninsula.
- A model developed to define groundwater protection zones for the Tadcaster brewery boreholes.
- A simple VKD test model used to test UCODE.

A summary of the tests and the differences in results produced by MF96 and MF-VKD is shown Table 2.

For the EPA tests there are no significant differences between MF96 and MF-VKD. For the USGS datasets the only significant difference occurs in stream flow calculations where known changes have been deliberately introduced to improve the MF-VKD code.

The GPZ model for the Tadcaster brewery boreholes was run four times:

1. MF-96 to produce full output files for comparison.
2. MF-VKD inactive.
3. MF-VKD active but with no variation in hydraulic conductivity with depth.
4. MF-VKD active and with hydraulic conductivity varying with depth.

The fourth simulation with VKD active and hydraulic conductivity varying with depth was performed using the auto-conversion option available in MF-VKD to introduce a variation in K with depth. In steady state this yields the same transmissivity values as those obtained with the original constant hydraulic conductivity model. The heads and flows predicted when hydraulic conductivity varies with depth were the same as those predicted using MF96 and MF-VKD without VKD active.

Particle tracking was performed on all four Tadcaster tests. The only significant difference in results is found when comparing MF-VKD with VKD active to the results of MF-96. Maximum spatial differences in particle tracks of 113.3 m were seen. These differences are due to the sensitivity of particle tracking to small rounding / precision errors which can put particles into different model cells and then transport them with different gradients and velocities due to slightly different steady state solutions being produced by the two versions of MODFLOW.

Two tests were used to explore whether differences in FORTRAN compiler cause discrepancies in model results. The Compaq and Salford FORTRAN compilers were used in the comparison to create the MF-VKD executable. The use of different compilers does not affect MF-VKD / MF-96 results.

One of the test models used in the original testing program for MF-VKD was employed to check whether MF-VKD can work with the optimisation and sensitivity analysis program UCODE. The test dataset and UCODE templates were modified and UCODE successfully calculated the sensitivity of VKD parameters. UCODE can be applied with MF-VKD and if necessary can explore the sensitivity of VKD parameters.

Table 2 List of tests and discrepancies identified in the results produced by MF96 and MF-VKD

Test Number	Test Name	Differences in results
1	US EPA problem 1	Insignificant (Type I)
2	US EPA problem 2	Insignificant (Type I)
3	US EPA problem 3	Insignificant (Type I)
4	US EPA problem 5	Insignificant (Type I)
5	US EPA problem 8	Insignificant (Type I)
6	US EPA problem 9	Insignificant (Type I)
7	US EPA problem 12	Insignificant (Type I)
8	US EPA problem 13	Insignificant (Type I)
9	US EPA problem 14	Insignificant (Type I)
10	US EPA problem 16	Insignificant (Type I)
11	US EPA problem 18	Insignificant (Type I)
12	US EPA problem 20	Insignificant (Type I)
13	USGS problem 1	Insignificant (Type I)
14	USGS problem 2	Significant differences in stream outflows due to correction in the accreted streamflow calculated in MF-VKD
15	USGS problem 3	Insignificant (Type I)
16	USGS problem 4	Insignificant (Type I)
17	USGS problem 5	Insignificant (Type I)
18	USGS problem 6	Insignificant (Type I)
19	USGS problem 7	Insignificant (Type I)
20	Wirral model (EA, 2002)	Insignificant (Type I)
21	Tadcaster model (EA, 1997) with MODPATH	Significant differences in pathlines (Type II) due to small differences in head and flow (Type I).
22	VKD test model (EA,2002) with UCODE	Insignificant (Type I)

4.2 Conclusions

The results produced for the series of tests performed using the unmodified and VKD version of MODFLOW show that the introduction of VKD does not alter the basic functionality of MODFLOW. The output files generated by MF96 and MF-VKD show insignificant numerical differences, which are due to the different output formats, precision settings and round-off errors associated with the calculations performed in the two programs.

The only significant differences emerge from:

- Test problem 14 (problem 2 of the USGS series) of the USGS suite, where the stream, STR, package is employed. The results reveal differences in the accretion profiles computed by MF96 and MF-VKD that are due to a small correction in the calculation of streamflows that was introduced in MF-VKD.
- Test problem 21 based on the GPZ model for the Tadcaster brewery boreholes. The .ptl files produced by MODPATH show differences in the particle positions, travel times and the number of cells particles cross along their pathline. These differences arise as a result of small discrepancies between the heads and flows calculated by the two different versions of MODFLOW. Whilst these discrepancies are not significant in themselves, the effect on particle locations can be significant. However, the differences are less than those associated with other modelling uncertainties, and do not indicate any problems with the validity of the VKD code.

Other tests performed with UCODE and different compilers show that MF-VKD can be compiled with different compilers without problems and that UCODE can be used with MF-VKD.

During a modelling project involving the use of MODFLOW-VKD that the Environment Agency undertook at the time of the further testing described in this report, a problem was found in the MODFLOW-VKD code. This problem occurs when both confined and unconfined storage are used in the model domain. Upon close analysis of this problem, WMC discovered that if the point of inflection on the VSD (variable unconfined storage with depth) profile is set above the top elevation of the MODFLOW layer, then the unconfined storage value is used when the confined S should be used. This error was corrected and WMC provided the Environment Agency with the revised code.

4.3 Recommendations

The use of MF-VKD rather than MF96 for simple non-VKD models may require small modifications to the input data files. For the tests described in this report, such modifications consist only in removing comments in the first line of the .BCF file. Similarly, small modifications to the format of input files may be necessary when running versions of MF-VKD created with different FORTRAN compilers. These modifications can be viewed in the test data files included in the CD accompanying the revised version of the User Guide for MODFLOW-VKD.

The magnitude of the discrepancies in the pathlines and travel times produced by MODPATH when used in combination with MF96 and MF-VKD are the result of small differences in cell-by-cell flows due to numerical round-off errors.

Particle tracking with MODPATH on a model with the VKD function active must be interpreted with great care. The velocities used to define pathlines are depth-averages within a layer and are not a full reflection of the VKD function. Since the pathlines from particle tracking with VKD active using MODPATH are inaccurate, the results should be viewed with much care. However, given the magnitude of other uncertainties in assumptions underlying particle tracking, such as a continuous porous medium assumption in a Chalk aquifer, the additional uncertainty that VKD introduces to MODPATH pathlines may be relatively small. The Agency does not at present have plans to develop a VKD version of MODPATH. It does plan to issue further guidance on Groundwater Protection Zone delineation where MODFLOW VKD regional models exist.

REFERENCES

Andersen, P.F., 1993, *A manual of instructional problems for the USGS MODFLOW model*. US Environmental Protection Agency Report EPA/600/R-93/010.

Environment Agency, 1997, *Tadcaster Groundwater Protection Zones*. WMC Report 1345/R1 prepared for the Environment Agency, Northeast Region.

Environment Agency, 2002a, *Enhancements to MODFLOW – Variation in hydraulic conductivity and storage with depth*. WMC Report 1621/R1 prepared for the Environment Agency, National Groundwater and Contaminated Land Centre, Project NC/00/23.

Environment Agency, 2003, *Enhancements to MODFLOW – User guide for MODFLOW-VKD – A modified version of MODFLOW-96 to include variations in hydraulic properties with depth*. WMC Report 1621/R3 prepared for the Environment Agency, National Groundwater and Contaminated Land Centre, Project NC/00/23.

Fenske, J.P., Leake, S.A., Prudic, D.E., 1996, *Documentation of a computer program (RES1) to simulate leakage from reservoirs using the modular finite-difference ground-water flow model (MODFLOW)*, U.S. Geological Survey Open-File Report 96-364, 58 p. Available at <http://water.usgs.gov/software/modflow-96.html>.

Harbaugh, A.W., and McDonald, M.G., 1996, *User's documentation for MODFLOW-96, an update to the U.S. Geological Survey modular finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 96-485*, 56 p. Available at <http://water.usgs.gov/software/modflow-96.html>.

Leake, S.A., Leahy, P.P., Navoy, A.S., 1994, *Documentation of a computer program to simulate transient leakage from confining units using the modular finite-difference ground-water flow model*, U.S. Geological Survey Open-File Report 94-59, 77 p. Available at <http://water.usgs.gov/software/modflow-96.html>.

Leake, S.A., and Lilly, M.R., 1997, *Documentation of a computer program (FHB1) for assignment of transient specified-flow and specified-head boundaries in applications of the modular finite-difference ground-water flow model (MODFLOW)*, U.S. Geological Survey Open-File Report 97-571, 56 p. Available at <http://water.usgs.gov/software/modflow-96.html>.

Leake, S.A., and Prudic, D.E., 1997, *Documentation of a computer program to simulate aquifer-system compaction using the modular finite-difference ground-water flow model*, U.S. Geological Survey Techniques of water resources investigation, Book 6, Chapter A2, 74 p. Available at http://water.usgs.gov/pubs/twri/twri6a2/pdf/TWRI_6-A2.pdf.

- McDonald, M.G., Harbaugh, A.W., Orr, B.R., Ackerman, D.J., 1991, Open-File Report 91-536, 103 p.
- Osiensky, J.L. and Williams, R.E., 1997, *Potential Inaccuracies in MODFLOW Simulations Involving the SIP and SSOR Methods for Matrix Solution*. Groundwater, Volume 35, No. 2.
- Poeter, E.P. and Hill, M.C., 1998, *Documentation of UCODE, a computer code for universal inverse modelling*. U.S. Geological Survey Water-Resources Investigations Report 98-4080, 116 p.
- Pollock, D.W., 1994, *User's Guide for MODPATH/MODPATH-PLOT, Version 3: A particle tracking post-processing package for MODFLOW, the U.S. Geological Survey finite-difference ground-water flow model*. U.S. Geological Survey Open-File Report 94-464, 6 ch. Available at <http://water.usgs.gov/software/modpath.html>
- Prudic, D.E., 1988, *Documentation of a computer program to simulate stream-aquifer relations using a modular finite-difference ground-water flow model*, Open-File Report 88-729, 119 p.
- Taylor, A.B., Hayes, P.J., Hulme, P.J., 2002, *Examination of Groundwater Flow Model Sensitivity Analysis and Parameter Optimisation using UCODE, prepared for the Environment Agency, National Groundwater and Contaminated Land Centre, Project NC/01/60*.

APPENDIX A
Results of the test problems

List of test problems

Test number	Test name	Description
1	US EPA problem 1	The Theis solution
2	US EPA problem 2	Anisotropy
3	US EPA problem 3	Artesian-water table conversion
4	US EPA problem 5	Mass balance
5	US EPA problem 8	Grid and time stepping considerations
6	US EPA problem 9	Calibration and prediction
7	US EPA problem 12	Leaky aquifers
8	US EPA problem 13	Solution techniques and convergence
9	US EPA problem 14	Head dependent boundary conditions
10	US EPA problem 16	Evapotranspiration
11	US EPA problem 18	Cross-sectional simulations
12	US EPA problem 20	Application to a hazardous waste site
13	USGS problem 1	Storage depletion (use of inter-bed storage, IBS1, package, which simulates storage changes and compaction in fine-grained beds and confining beds. Used to reproduce aquifer compaction and land subsidence)
14	USGS problem 2	Example problem in OFR 88-729 (use of stream, STR, package)
15	USGS problem 3	Example problem in TWRI 6-A1
16	USGS problem 4	Example problem in OFR 91-536
17	USGS problem 5	Example problem 1 in OFR 94-59 (use of transient leakage, TLK1, package to simulate storage depletion in confining beds)
18	USGS problem 6	Example problem in OFR 96-364 (use of reservoir, RES1, package to simulate leakage from a reservoir)
19	USGS problem 7	Example problem in OFR 97-571 (use of transient specified flow and specified head boundary, FHB1, package)
20	Wirral117tv	Wirral regional model
21	Tad401	Tadcaster model (EA, 1997) with MODPATH
22	VKD19-tv	VKD test model (EA, 2002a) with UCODE

Test Problem 1					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
US EPA problem 1 [modflmn.pdf, 1-1]	The Theis solution (Part a)	Confined model, 1 layer, 19 rows, 19 cols with mesh spacing reduction around pumping well in centre of grid. One stress period of 1 day and 20 time steps.	pr1a	.WEL .SIP .OPC	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)	
None		None		Set BOT = -100 m and TOP = -99 m in order to reproduce strictly confined conditions. Kbase=T, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1=Sf2, VSMID=BOT, VSGRAD=1, VS MAX=1.	
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
Balance residuals in volumetric budget (Type I)	Type I	Balance residuals, storage changes and total inflows in volumetric budget (Type I)	Type I	Balance residuals, storage changes and total inflows in volumetric budget (Type I)	Type I

Test Problem 2					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
US EPA problem 2 [modflmn.pdf, 2-1]	Anisotropy (Part b)	Same as problem 1, with one quadrant of model grid (pumping well in node [1,1]) and anisotropy ratio Ty/Tx of 0.1	pr2b	.WEL .SIP .OPC	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)	
None		Eliminate comment on 1 st line of .BCF file.		Set BOT = -100 m and TOP = -99 m in order to reproduce strictly confined conditions. Kbase=T, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1=Sf2, VSMID=BOT, VSGRAD=1, VS MAX=1.	
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
Balance residuals in volumetric budget (Type I)	Type I	Maximum head changes (Type I)	Type I	Balance residuals in volumetric budget and maximum head changes (Type I)	Type I

Test Problem 3					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
US EPA problem 3 [modflmn.pdf, 3-1]	Artesian-water table conversion	Confined-unconfined model with constant T and variable S (LAYCON=2), 1 layer, 26 rows, 26 cols with mesh spacing reduction towards pumping well in node [1,1]. One stress period of 100 days and 25 time steps.	pr3	.WEL .SIP .OPC	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)	
None		None		Not possible to reproduce LAYCON conditions with LAYCON 4 or 5. Run not executed.	
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
Flow terms in volumetric budget and elapsed times (Type I)	Type I	N/A	N/A	N/A	N/A

Test Problem 4					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
US EPA problem 5 [modflmn.pdf, 5-1]	Mass balance	Confined model, 1 layer, 7 rows, 7 cols, specified heads along row 1 and column 7. One stress period of 365 days and 5 time steps.	pr5	.RCH .SIP .OPC	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)	
None		Eliminate comment on 1 st line of .BCF file.		Set BOT = -100 m and TOP = -99 m in order to reproduce strictly confined conditions. Kbase=T, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1=Sf2, VSMID=BOT, VSGRAD=1, VS MAX=1.	
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
Flow terms in volumetric budget (Type I)	Type I	Flow terms in volumetric budget and drawdowns (Type I)	Type I	Flow terms in volumetric budget and drawdowns (Type I)	Type I

Test Problem 5					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
US EPA problem 8 [modflmn.pdf, 8-1]	Grid and time stepping considerations (Part a)	Confined model, 1 layer, 4 rows, 4 cols, specified heads (set with GHB) along edge of one side. One stress period of 20 days and 10 time steps.	p8a	.WEL .GHB .SIP	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)	
None		Eliminate comment on 1 st line of .BCF file.		Set BOT = -100 m and TOP = -99 m in order to reproduce strictly confined conditions. Kbase=T, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1=Sf2, VSMID=BOT, VSGRAD=1, VSMAX=1.	
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
Flow terms in volumetric budget (Type I)	Type I	Flow terms in volumetric budget (Type I)	Type I	Flow terms in volumetric budget (Type I)	Type I

Test Problem 6					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
US EPA problem 9 [modflmn.pdf, 9-1]	Calibration and prediction (Part a)	Confined model, 1 layer, 15 rows, 15 cols, with river crossing along west-east direction. Steady state simulation.	p9a,b	.WEL .RIV .RCH .SIP	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)	MODFLOW-VKD VKD active (C)		
None		Eliminate comment on 1 st line of .BCF file.	Set BOT = -100 m and TOP = -99 m in order to reproduce strictly confined conditions. Kbase=T, VMID=BOT, VKGRAD=1, VKMAX=1.		
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
None	Type I	None	Type I	None	None

Test Problem 7					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
US EPA problem 12 [modflmn.pdf, 12-1]	Leaky aquifers (Part a)	10 confined layers (1 layer for upper aquifer, 7 layers for aquitard, 2 layers for lower aquifer), 25 rows, 25 cols with mesh spacing reduction towards pumping well in nodes [9,1,1] and [10,1,1]. One stress period of 787900 s and 30 time steps.	p12a	.WEL .SIP .OPC	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)	
None		None		Set BOT of 10 layers from -500 to -509 m and TOP from -499 to -508 m in order to reproduce strictly confined conditions. Kbase=T, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1=Sf2, VSMID=BOT, VSGRAD=1, VSMAX=1 in all layers.	
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
Flow terms in volumetric budget and elapsed times (Type I)	Type I	Drawdowns, flow terms in volumetric budget and elapsed times (Type I)	Type I	Drawdowns and flow terms in volumetric budget (Type I)	Type I

Test Problem 8					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
US EPA problem 13 [modflmn.pdf, 13-1]	Solution techniques and convergence (Part a and b)	3 layers (layer 1 unconfined, layer 2 and 3 confined), 10 rows, 15 cols with specified head along east side in layer 1. Steady-state simulation.	p13a,b,c	.RCH .SIP .SOR .OC (created) .PCG (created)	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)	
Increase MXITER in .SIP for sip solver to achieve convergence.		Increase MXITER in .SIP for sip solver to achieve convergence. Eliminate comment on 1 st line of .BCF file.		Increase MXITER in .SIP for sip solver to achieve convergence. Set BOT of layer 2 and 3 from -501 to -502 m and TOP of layer 2 and 3 from -500 to -501 m in order to reproduce strictly confined conditions. Kbase=K in layer 1, Kbase=T in layer 2 and 3, VMID=BOT, VKGRAD=1, VKMAX=1 in all layers.	
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
None	Type I	None	Type I	None	Type I

Note:

This problem was run using both the SIP and PCG2 solvers with essentially identical results being obtained

Test Problem 9					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
US EPA problem 14 [modflmn.pdf, 14-1]	Head dependent boundary conditions (Part a, c and d considered at once)	Unconfined model, 1 layer, 7 rows, 7 cols with uniform mesh spacing, pumping well in node [1,1]. Set a river, drains and evt along col 4. One stress period of 365 days and 20 time steps.	p14	.WEL .DRN .RIV .ET .SIP .OPC	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)	
None		Eliminate comment on 1 st line of .BCF file.		Set Kbase=K, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1, VSMID=BOT, VSGRAD=1, VSMAX=1.	
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
Flow terms in volumetric budget (Type I)	Type I	Flow terms in volumetric budget (Type I)	Type I	Flow terms in volumetric budget, maximum head changes and heads (Type I)	Type I

Test Problem 10					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
US EPA problem 16 [modflmn.pdf, 16-1]	Evapotranspiration (Part a)	Unconfined model, 1 layer, 20 rows, 18 cols with specified heads in zone to the east. One stress period of 1 day and 1 time step.	p16a	.ET .RCH .SIP .OPC (created)	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)	MODFLOW-VKD VKD active (C)		
None		Eliminate comment on 1 st line of .BCF file.	Set Kbase=K, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1, VSMID=BOT, VSGRAD=1, VSMAX=1.		
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
None	Type I	None	Type I	None	None

Test Problem 11						
Reference		Name		Description	Dataset Root Name	MF optional files employed
US EPA problem 18 [modflmn.pdf, 18-1]		Cross-sectional simulations (Part b)		Vertical section (1 row), 6 layers (layer 1 is unconfined, other layers are convertible), 27 cols, specified head in layer 1, 2 and 3 reproduce river, spec. heads in layer 6 reproduce leakage. Steady-state simulation.	p18	.RCH .SOR .OPC
Change to input data files						
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)		
None		Eliminate comment on 1 st line of .BCF file.		Set Kbase=K, VMID=BOT, VKGRAD=1, VKMAX=1 in all layers.		
Comparison of output files – Difference types						
AB		AC		BC		
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files	
None	None	Constant head flows in volumetric budget (Type I)	None	None	None	

Test Problem 12											
Reference		Name		Description				Dataset Root Name		MF optional files employed	
US EPA problem 20 [modflmn.pdf, 20-1]		Application to a hazardous waste site (Part a, b and d)		Unconfined model, 1 layer, 39 rows, 37 cols with mesh spacing reduction in landfill site, a drain is present. Steady-state simulation to produce the initial heads for a time-variant simulation with one stress period of 30.8 years and 20 time steps.				p20a,b,d,ba,bb,b,bd a,bdb		.DRN .RCH .SIP .PCG (created) .OPC	
Change to input data files											
MODFLOW 96 (A)				MODFLOW-VKD VKD inactive (B)				MODFLOW-VKD VKD active (C)			
Copy head matrix generated in the steady-state simulation into the .BAS file used in the time-variant run.				Copy head matrix generated in the steady-state simulation into the .BAS file used in the time-variant run.				Copy head matrix generated in the steady-state simulation into the .BAS file used in the time-variant run. Set Kbase=K, VMID=BOT, VKGRAD=1, VKMAX=1 and Sbase=Sf1, VSMID=BOT, VSGRAD=1, VSMAX=1 in time-variant run.			
Comparison of output files – Difference types											
AB				AC				BC			
.OUT files		.DAT files		.OUT files		.DAT files		.OUT files		.DAT files	
SS	TV	SS	TV	SS	TV	SS	TV	SS	TV	SS	TV
None	Flow terms in volumetric budget (Type I)	Type I	Type I	None	Flow terms in volumetric budget, maximum head changes, drawdowns and heads (Type I)	Type I	Type I	None	Flow terms in volumetric budget, maximum head changes, drawdowns and heads (Type I)	None	Type I

Note:

This problem was run using both the SIP and PCG2 solvers with essentially identical results being obtained

Test Problem 13							
Reference	Name		Description	Dataset Root Name	MF optional files employed		
USGS problem 1 [TWRI Book 6, Chapter A2]	Storage depletion (use of inter-bed storage, IBS1, package, which simulates storage changes and compaction in fine-grained beds and confining beds. Used to reproduce aquifer compaction and land subsidence)		2 confined layers (layer 1 has interbed storage), 10 rows, 12 cols. Three stress periods of 1000 days and 10 time steps.	IBS	.SIP .OC .IBS		
Change to input data files							
MODFLOW 96 (A)	MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)	MODFLOW-VKD (Compaq compiled) VKD active (C1)			
Added comments in .IBS file	None		Set BOT of layer 1 and 2 from -501 to -502 m and TOP of layer 2 and 3 from -500 to - 501 m in order to reproduce strictly confined conditions. Kbase=T, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1=Sf2, VSMID=BOT, VSGRAD=1, VS MAX=1 in both layers.	Set BOT of layer 1 and 2 from - 501 to -502 m and TOP of layer 2 and 3 from -500 to -501 m in order to reproduce strictly confined conditions. Kbase=T, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1=Sf2, VSMID=BOT, VSGRAD=1, VS MAX=1 in both layers. Replace tabs with spaces in IBS.IBS file			
Comparison of output files – Difference types							
AB		AC		BC		CC1	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
Flow terms in volumetric budget (Type I)	Type I	Flow terms in volumetric budget and maximum head changes (Type I)	Type I	Flow terms in volumetric budget and maximum head changes (Type I)	Type I	None	Type I

Test Problem 14							
Reference	Name	Description	Dataset Root Name	MF optional files employed			
USGS problem 2 [OFR 88-729]	Example problem in OFR 88-729 (use of stream, STR, package)	Confined model, 1 layer, 6 rows, 6 cols, a stream crosses the modelled area. One stress period of 15 days and 3 time steps.	STR	.SIP .OC .STR			
Change to input data files							
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)		MODFLOW-VKD (Compaq compiled) VKD active (C1)	
None		None		Set BOT = -501 m and TOP = -500 m, in order to reproduce strictly confined conditions. Kbase=T, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1=Sf2, VSMID=BOT, VSGRAD=1, VSMAX=1.		Set BOT = -501 m and TOP = -500 m, in order to reproduce strictly confined conditions. Kbase=T, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1=Sf2, VSMID=BOT, VSGRAD=1, VSMAX=1.	
Comparison of output files – Difference types							
AB		AC		BC		CC1	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
Flow terms in volumetric budget, heads and drawdowns (Type I)	Type II At time step 3, stream outflow [m ³ /day] at nodes: [2,3]. A=5.11, B=2.27, %diff=77 [5,3]. A=1.79, B=0.99, %diff=58 [5,4]. A=9.20, B=5.25, %diff=55. See Note	Flow terms in volumetric budget, heads, drawdowns and maximum head changes (Type I)	Type II* At time step 3, stream outflow [m ³ /day] at nodes: [2,3]. A=5.11, B=2.27, %diff=77 [5,3]. A=1.79, B=0.99, %diff=58 [5,4]. A=9.20, B=5.25, %diff=55. See Note	None	None	None	Type I
Note: A discrepancy in stream outflows is expected in cells where more than one reach is defined, as a correction in the calculation of the accreted streamflow was introduced in the MF-VKD code. This is explained in detail in Section 3.2.3 of MF-VKD User Guide (EA, 2003).							

Test Problem 15					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
USGS problem 3 [TWRI Book 6, Chapter A1, Appendix D]	Example problem in TWRI 6-A1	3 layers (layer 1 unconfined, layer 2 and 3 confined), 15 rows, 15 cols, specified heads along one side in layer 1 and 2, drains and pumping wells are present. Steady-state simulation.	TWRI	.WEL .DRN .RCH .SIP .OC (created)	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)	MODFLOW-VKD VKD active (C)		
None		Eliminate comment on 1 st line of .BCF file.	Set BOT of layer 2 and 3 from -901 to -902 m and TOP of layer 2 and 3 from -900 to -901 m in order to reproduce strictly confined conditions. Kbase=K in layer 1, Kbase=T in layer 2 and 3, VMID=BOT, VKGRAD=1, VKMAX=1 in all layers.		
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
None	Type I	None	Type I	None	Type I

Test Problem 16					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
USGS problem 4 [OFR 91-536, not available on-line]	Example problem in OFR 91-536	2 layers (layer 1 unconfined, layer 2 confined), 10 rows, 15 cols, a river and two pumping wells are present. Two stress periods of 1 day and 1 time step each.	BCF2SS	.WEL .RIV .RCH .PCG .OC	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)	
None		None		Set BOT of layer 2 = -901 m and TOP of layer 2 = -900 m in order to reproduce strictly confined conditions. Kbase=K in layer 1, Kbase=T in layer 2, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1 in layer 1, Sbase=Sf1=Sf2 in layer 2, VSMID=BOT, VSGRAD=1, VSMAX=1 in both layers.	
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
None	Type I	None	Type I	None	None

Test Problem 17					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
USGS problem 5 [OFR 94-59]	Example problem 1 in OFR 94-59 (use of transient leakage, TLK1, package to simulate storage depletion in confining beds)	Vertical section (1 row), 4 layers (all layers confined), 13 cols, specified heads along model edges, storage of confining layers is reproduced. One stress period of 100 days and 40 time steps.	TLKP1	.TLK .SIP .OC	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)	
None		None		Set BOT of layers from -901 m to -904 m and TOP from -900 m to -903 m in order to reproduce strictly confined conditions. Kbase=T, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1=Sf2, VSMID=BOT, VSGRAD=1, VSMAX=1 in all layers.	
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
Flow terms in volumetric budget, (Type I)	Type I	Flow terms in volumetric budget and maximum head changes (Type I)	Type I	Flow terms in volumetric budget and maximum head changes (Type I)	Type I

Test Problem 18					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
USGS problem 6 [OFR 96-364]	Example problem in OFR 96-364 (use of reservoir, RES1, package to simulate leakage from a reservoir)	Confined model, 1 layer, 12 rows, 12 cols, general-head boundaries along the model edges, a reservoir is present. Three stress periods of 5 days and 5 time steps each.	RESTEST	.GHB .SIP. .OC .RES	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)	
None		None		Set BOT = -901 m and TOP = -900 m in order to reproduce strictly confined conditions. Kbase=T, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1=Sf2, VSMID=BOT, VSGRAD=1, VS MAX=1.	
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
Storage flow terms in volumetric budget, (Type I)	Type I	Storage flow terms in volumetric budget, (Type I)	Type I	Flow terms in volumetric budget, (Type I)	Type I

Test Problem 19					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
USGS problem 7 [OFR 97-571]	Example problem in OFR 97-571 (use of transient specified flow and specified head boundary, FHB1, package)	1 layer, 3 rows, 10 cols. Three stress periods of 400, 200, 400 days and 10, 4, 6 time steps respectively.	FHB	.SIP .OC .FHB	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)	
None		None		Set BOT = -901 m and TOP = -900 m in order to reproduce strictly confined conditions. Kbase=T, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1=Sf2, VSMID=BOT, VSGRAD=1, VSMAX=1.	
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
Flow terms in volumetric budget (Type I)	Type I	Flow terms in volumetric budget (Type I)	Type I	Flow terms in volumetric budget (Type I)	Type I

Test Problem 20					
Reference	Name	Description	Dataset Root Name	MF optional files employed	
Examination of Groundwater Flow Model Sensitivity Analysis and Parameter Optimisation using UCODE, NGWCLC Project NC/01/60, Chapter 4	Wirral regional model	1 layer (convertible with variable T), 122 rows, 90 cols, river cells located along the coast to limit inflow, pumping wells with large abstraction. 348 stress periods of one-month and 1 time step each.	wirral117tv	.RCH .WEL .RIV .STR (dummy) .OC .PCG	
Change to input data files					
MODFLOW 96 (A)		MODFLOW-VKD VKD inactive (B)		MODFLOW-VKD VKD active (C)	
None		None		Set Kbase=K, VMID=BOT, VKGRAD=1, VKMAX=1, Sbase=Sf1=Sf2, VSMID=BOT, VSGRAD=1, VSMAX=1.	
Comparison of output files – Difference types					
AB		AC		BC	
.OUT files	.DAT files	.OUT files	.DAT files	.OUT files	.DAT files
Flow terms in volumetric budget, heads, drawdowns and maximum head changes (Type I)	Type I	Flow terms in volumetric budget, heads, drawdowns and maximum head changes (Type I)	Type I	Flow terms in volumetric budget and maximum head changes (Type I)	Type I
<i>Note: Cell-by-cell flows, heads and drawdowns are printed only in 1st and last stress period in order to reduce the size of the .OUT and .CBB files and allow comparison with UltraEdit-32©.</i>					

Test Problem 21				
Reference	Name	Description	Dataset Root Name	MF optional files employed
Tadcaster Groundwater Protection zones. WMC Report 1345/R1.	Tadcaster GPZ flow and particle tracking model	1 unconfined layer, 148 rows, 194 cols, general-head boundaries along Northeast edge representing lateral continuation of aquifer, river cells representing the River Wharfe, Bramham Beck and Cock Beck, pumping wells with large abstraction. Steady-state simulation.	Tad401 (Modflow files) Tad401p (Modpath files)	.WEL .RCH .RIV .GHB .OC .PCG
Change to input data files				
MODFLOW 96 (A)	MODFLOW-VKD VKD inactive (B)	MODFLOW-VKD VKD active (C)	MODFLOW-VKD VKD active, variable K (D)	
None	None	Set Kbase=K, VMID=BOT, VKGRAD=1, VKMAX=1.	Using the auto-conversion option, set Kbase=K, thickness of upper zone = 5, VKGRAD=1, VKMAX=3.	
Comparison of output files – Difference types				
AB	.OUT files	None		
	.DAT files	Type I		
	.PTL files	Type I		
AC	.OUT files	None		
	.DAT files	Type I		
	.PTL files	Type I		
AD	.OUT files	Flow terms in volumetric budget, heads and drawdowns (Type I)		
	.DAT files	Max head diff = -0.018 m, Max cbc diff = -0.0367 m ³ /day (Type I)		
	.PTL files	Max travel time diff = 5.4 %, Max diff in X, Y and Z coord = 92.11, 37.74 and 3.3 m respectively.		
BC	.OUT files	None		
	.DAT files	None		
	.PTL files	None		
BD	.OUT files	Flow terms in volumetric budget, heads and drawdowns (Type I)		
	.DAT files	Max head diff = -0.018 m, Max cbc diff = -0.0367 m ³ /day (Type I)		
	.PTL files	Type I		
CD	.OUT files	Flow terms in volumetric budget, heads and drawdowns (Type I)		
	.DAT files	Max head diff = -0.018 m, Max cbc diff = -0.0367 m ³ /day (Type I)		
	.PTL files	Type I		

APPENDIX B
Contents of the CD included in the revised version of the User
Guide for MODFLOW-VKD

The directory structure of the deliverables related to the project VKD further testing - Phase 1 (Groundwater Technical Services Contract #11589) is shown below. This structure is also detailed in the file `readme_deliverables.txt`.

> **Reports & Documentation:** directory containing the updated User Guide and all MODFLOW-VKD reports in PDF format

> **Software:** directory containing the programs MF96.exe, MF-VKD6.exe (including source code), MF-VKD6-Compaq.exe (compiled with the Compaq FOTRAN compiler) and the utilities heads2gv.exe, cbc2gv.exe, cbc2dos.exe employed to compare the .HDS and .CBB files produced in the tests

> **Example datasets from further testing:**

> **USEPA_Tests:** directory containing the EPA instructional problems for MODFLOW used for VKD testing. The I/O files for each problem are stored in separate sub-directories. Each sub-directory is named according to the problem number and includes the following:

- comparison files (.TXT) for the .OUT files and the ASCII version (.DAT) of the .CBB files

- comparison spreadsheets (.XLS) for the ASCII version (.DAT) of the .CBB files, for the tests where comparison files reveal several discrepancies (problems 1,2,12,14,20TV)

- > **Mf96(A):** directory containing the I/O files of the test performed with MF96

- > **vkd_inact(B):** directory containing the I/O files of the test performed with MF-VKD (VKD function inactive)

- > **vkd_act(C):** directory containing the I/O files of the test performed with MF-VKD (VKD function active)

> **USGS_Tests:** directory containing the USGS MODFLOW tests used for VKD testing. The I/O files for each problem are stored in separate sub-directories. Each sub-directory is named according to the problem number and includes the following:

- comparison files (.TXT) for the .OUT files and the ASCII version (.DAT) of the .CBB files

- comparison spreadsheets (.XLS) for the ASCII version (.DAT) of the .CBB files, for the tests where comparison files reveal several discrepancies (problems 1,2,5)

- > **Mf96(A):** directory containing the I/O files of the test performed with MF96

- > **vkd_inact(B):** directory containing the I/O files of the test performed with MF-VKD (VKD function inactive)

- > **vkd_act(C):** directory containing the I/O files of the test performed with MF-VKD (VKD function active)

- > **vkd_act_Compacq(C1)** [in problems 1 and 2]: directory containing the I/O files of the test performed with MF-VKD compiled with the FORTRAN Compaq compiler (VKD function active)

> **Wirral_model:** directory containing I/O files for the Wirral MODFLOW model ('wirral117tv' root name). This directory contains the following:

- comparison files (.TXT) for the .OUT files and the ASCII version (.DAT) of the .CBB files

- comparison spreadsheets (.XLS) for the ASCII version (.DAT) of the .HDS and .CBB files

- > **Mf96(A):** directory containing the I/O files of the test performed with MF96

- > **vkd_inact(B):** directory containing the I/O files of the test performed with MF-VKD (VKD function inactive)

- > **vkd_act(C):** directory containing the I/O files of the test performed with MF-VKD (VKD function active)

> **Tadcaster_model**: directory containing I/O files for the MODFLOW and MODPATH Tadcaster GPZ model ('tad401' root name). This directory contains the following:

- comparison files (.TXT) for the .OUT files and the ASCII version (.DAT) of the .CBB files
- comparison spreadsheets (.XLS) for the ASCII version (.DAT) of the .HDS, .CBB files and for the .PTL files

> **Mf96(A)**: directory containing the I/O files of the test performed with MF96 and MODPATH

> **vkd_inact(B)**: directory containing the I/O files of the test performed with MF-VKD (VKD function inactive) and MODPATH

> **vkd_act(C)**: directory containing the I/O files of the test performed with MF-VKD (VKD function active) and MODPATH

> **vkd_act_Teq(D)**: directory containing the I/O files of the test performed with MF-VKD (VKD function active and depth-dependent K) and MODPATH

> **Additional documentation**: directory containing the reports that describe some of the tests

> **Spreadsheets and utilities developed by various consultants on different projects where MODFLOW-VKD has been used**

APPENDIX G
Independent review of the MODFLOW VKD code

INDEPENDENT REVIEW OF THE MODFLOW VKD CODE

**David Lerner, Groundwater Protection and Restoration Group, University of Sheffield,
July 2003**

SUMMARY

The code development and testing have been well carried out, and the code should be released for use in flow modelling. I have three recommendations:

- 1) The results of the use of the code in further field situations are reviewed.
- 2) Further attempts are made to understand the causes of the difficulties with the particle tracking when VKD is present but not operational. However efforts to improve MODPATH should be concentrated on issues of high significance to the Environment Agency, such as fractured rocks.
- 3) Contact is made with the code custodians, as it would be useful to have VKD recognised as an official variant on MODFLOW, and achieve forward compatibility.

INTRODUCTION

This is my response to The Environment Agency's request (email from Sarah Evers 28th Mar 03 and EA order 032029353 of 16th June 03) to review several reports on the above project. I have the following documents:

- a. Representation of the variation of hydraulic conductivity with saturated thickness in MODFLOW. Stages I & II - Code changes and testing against Birmingham University code (NC/99/67, August 1999, ISBN 0 857 051947). Paper and electronic copies of report, electronic copy of appendices.
- b. Representation of the variation of hydraulic conductivity with saturated thickness in MODFLOW. Stage III - Investigation using South West Chilterns model. (NC/99/67, July 2000, ISBN 1 857 05360 5). Paper copy received late June.
- c. Enhancements to MODFLOW - Variations in hydraulic conductivity and storage with depth. (NC/00/23, March 2002, ISBN 1 857 05765 1). Part copy received late June, full copy received late July.
- d. Enhancements to MODFLOW - User guide for MODFLOW-VKD - A modified version of MODFLOW-96 to include variations in hydraulic properties with depth. (NC/00/23, March 2002, ISBN 1 857 05766 X). Paper copy received late June.
- e. Further Testing of the MODFLOW VKD – Draft version (NC/XXXXXX, April 2003, in preparation). Electronic copy.
- f. Responses to a draft review from Sarah Evers (EA) and Phil Hayes (WMC).

Objectives of the review

The objective of the review, as specified in the tender documents, was "To provide independent review of the MODFLOW VKD code and of the further testing of the MODFLOW VKD code". (A second objective "To test VKD functionality in a way which is appropriate" was excluded from the tender.) I have considered the following questions in reviewing the documents:

- Has the approach adopted been logical and stepwise?
- Has sufficient care been taken in checking the results?
- Does the evidence show that the code performs as required?
- Were the test cases suitable?
- Should any further test be conducted?
- Any other comments.

REVIEW

Has the approach adopted been logical and stepwise?

Yes. The changes to the code were made in two major batches (Reports A and C). Within each batch, the changes were made in increments, tested individually, and the changes and tests were well documented.

Has sufficient care been taken in checking the results?

Yes. The checking was sufficiently detailed to identify errors in the original BHM code, and to spot oddities in the data in the SW Chilterns model. The consultants pursued the detail of any differences between models or unexpected results until they either had an explanation or made corrections.

Does the evidence show that the code performs as required?

Yes. The VKD code reproduces the results of the BHM code, which was the initial objective. It also is compatible with the unchanged MODFLOW.

The VSD option was found to make the code less stable, and there were difficulties in finding solutions with the complex multi-layer case. These are not surprising, all groundwater codes have some scenarios which are very difficult to find solutions for, and they need to be nursed through. The issues have been clearly identified in the documentation.

Problems were found with matching particle tracking results. I agree this is probably due to rounding errors, but this has not been proven. If true, it shows that particle tracking is very sensitive to small changes in parameter values, especially for time-of-travel-zones, and the resulting uncertainties should be recognised.

Were the test cases suitable?

The basic tests in A were OK, that is fairly simple but reasonable first steps. The tests against the USGS and field-based examples in E were sensible choices for checking conformity with the original MODFLOW. The results were adequately summarised.

Only two examples of the code's use with real field problems were presented, the SW Chilterns and Tadcaster models. The Chilterns case was used to demonstrate the VKD capability, and no attempt was made to re-calibrate the model. It could be argued that the VKD model was a poorer fit than the original, particularly on streamflow. The example demonstrates that the code works, but does not make a case that it was useful; only the former was intended. The Tadcaster case was principally used to test MODPATH, and was suitable for the purpose.

Four other field cases were modelled (Minram, Itchen, Bourne, Kennet). These will be reviewed separately, based on presentations to be made at a seminar in October 2003.

Overall, a sufficient and suitable range of test cases has been used.

Should any further tests be conducted?

No. I can see no obvious issues to tackle, except for the particle tracking problem. The next stage is to use the code in earnest on real field problems, demonstrate that the underlying conceptual model works well, and that the code is stable. The modellers will need to aware, as always, that unexpected errors could arise, and should build in some resources for careful checking of results. See below on the particle tracking issue.

Any other comments.

There are a few typos and missing references in the reports, but no major errors were found. Report E was still in draft.

Some problems outside the remit of the project (e.g. stream package) were detected and corrected. Some useful diagnostic outputs were added.

There is no evidence of contact with the code custodians, as recommended in Report A. I recommend this done, as it would be useful to have this recognised as an official variant on MODFLOW, and help to achieve forward compatibility.

Chapter 8 of the User Guide is important, as it gives help in how to approach a modelling problem rather than just dealing with the mechanics of data entry.

The differences encountered with particle tracking require some investigation, although there may not be any solution. If they are due to rounding errors, then remember that there are approximations in the way MODPATH handles velocity interpolation, which are at least as significant and no further action is needed. If changes are needed to the code to handle vertical variations in velocity, then the proposed approach in Report E is too simple, and work will need to start from a clear conceptual model of the hydrogeology and its representation in the code. For example, how is velocity handled in a cell with a well, where the vertical elevation of the exit point at the well is unknown? However, it is the EA's intention to concentrate resources on other issues related to SPZs (fractured rock, recharge). These are significant issues that should take precedence.

APPENDIX H
Summary of MODFLOW VKD version history

- MF-VKD1.exe (Oct 2001) Previous release of software
- MF-VKD2.exe (Jan 2003) Fixed bug so that confined storage values were used when heads rise above the top (when LAYCON = 5)
- MF-VKD3.exe (May 2003) Allow VKGRAD and VKMAX to be input as absolute values (rather than just as multiples of Kbase)
- MF-VKD4.exe (May 2003) Allow output of calculated internodal transmissivity values to a binary output file (rather than just as text to the listing file)
- MF-VKD5.exe (May 2003) Allow VSGRAD and VSMAX to be input as absolute values (rather than just as multiples of Kbase)
- MF-VKD6.exe (May 2003) Change to use double precision variables (including binary output) (makes VSD calculations more likely to converge)
- MF-VKD7.exe (Jun 2003) Fixed bug so that zero values entered for K or S zones would not produce a divide by zero error when specifying absolute values for VKGRAD, etc.