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Testing of particle tracking with MODFLOW-VKD

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Steve Killeen

Steve Killeen Head of Science

Executive Summary

This report details an investigation into the use of particle tracking with the Environment Agency's variable hydraulic conductivity with depth groundwater model, MODFLOW-VKD. MODFLOW-VKD represents variable hydraulic conductivity within single model layers of the Chalk.

MODPATH, the particle tracking code most commonly used with MODFLOW, does not take into account changes of hydraulic conductivity with depth. Particle tracking is used primarily by the Agency for definition of Source Protection Zones (SPZs).

This project investigates some possible ways particle tracking can be performed using MODPATH with MODFLOW-VKD models and suggests a forward for particle tracking with VKD models.

Time Instant Steady State (TISS) runs for the extreme groundwater levels (highest and lowest) produce theoretical extremes for capture zones. But these give unrealistic particle tracks so that the SPZs do not reflect the time variant nature of the the real system, particularly in the Chalk. Hence TISS models are not recommended for defining SPZs.

It is possible to correct particle tracks for the effects of VKD in steady state models without modifications to MODPATH. The correction technique could be incorporated into MODPATH for use with time variant models, but this would require considerable work (£15,000-30,000).

In an isotropic, steady state, model VKD only affects the magnitude of the velocity vector, therefore the speed of particles increases but there is no change in particle direction. The 50-day and 400-day capture zones are typically larger for VKD corrected runs. The total capture zone remains the same.

Time variant particle tracking is probably more important in terms of defining SPZs than the full incorporation of VKD into MODFLOW. A method has been developed to produce a probabilistic capture zone plot for an abstraction. Full account is taken of the seasonal variations in recharge, heads and velocities within the aquifer. The technique is equally applicable to aquifers other than the Chalk.

There are some unresolved issues with the technique including: 1) The 50 and 400-day time of travel zones have not been defined, although this should be possible; 2) VKD is not fully taken into account because particle tracking is performed using time variant depth averaged velocities.

Contents

Introduction

1.1 Background

This report details an investigation into the use of particle tracking with the Environment Agency's variable hydraulic conductivity with depth groundwater model, MODFLOW-VKD (Environment Agency 2003). MODFLOW-VKD permits the representation of variable hydraulic conductivity within single model layers. It was specifically developed to represent Chalk aquifers where the hydraulic conductivity of the aquifer can vary significantly within the zone of groundwater fluctuation.

MODPATH (Pollock 1994), the particle tracking code most commonly used with MODFLOW (Harbaugh and McDonald 1996), does not take into account changes of hydraulic conductivity with depth. This project investigates a number of potential ways particle tracking can be performed using MODPATH with MODFLOW-VKD models. The aim of the project is to explore the potential for inaccuracies if MODPATH is used with VKD models and, to the extent possible, outline ways forward for particle tracking with VKD models.

Particle tracking is used primarily by the Agency for definition of Source Protection Zones (SPZs). Whilst this project concentrates on SPZ delineation, the discussion and conclusions drawn are equally applicable to other uses of particle tracking.

1.2 Scope of work

The scope of work for the project is detailed in a letter to Sarah Evers dated 22nd June 2004. The project consists of 4 tasks:

- Task 1. Extract heads and cell-by-cell flows for steady state particle tracking at high and low groundwater conditions.
- Task 2. Perform particle-tracking simulations in steady state for the high and low groundwater conditions.
- Task 3. Conduct a correction to the paths/travel times taking VKD parameters into account using the techniques illustrated by Chris Jackson in the ZoomQ3D code.
- Task 4. Reporting of the influence of VKD on particle tracking and recommendations concerning its future use.

For practical particle tracking tests this project uses the Bourne and Nine Mile groundwater model developed by South West Region of the Agency in conjunction with WMC between 2002 and 2004 (WMC 2004). The Bourne model is a calibrated Regional model of the Chalk block to the north of Salisbury and includes the VKD function.

This report assumes that readers are familiar with MODFLOW-VKD, Environment Agency (the Agency) SPZ policy and MODPATH.

1.3 Additional work completed

In addition to the tasks outlined above, additional work was completed looking at the option of using time variant models for particle tracking. Given the large seasonal variation in groundwater levels and flows seen in Chalk aquifer systems, the use of steady state simulations for particle tracking is a poor approximation. The additional work completed has shown that there are several possibilities for time variant particle tracking that fully utilise time variant Regional models. The most promising of these is demonstrated to be capable of producing a probabilistic approach to SPZ delineation.

1.4 Structure of work

The second section of this report details the work undertaken for Tasks 1 and 2 of the scope of work, looking at steady state particle tracking at high and low groundwater conditions. This covers the methodology used for extracting heads from the Bourne model, the set-up of the steady state models and particle tracking.

Section 3 concerns Task 3, the ZOOPT correction for VKD and applying it to the steady state models from Task 2. Section 4 details time variant particle tracking as an additional potential method for SPZ delineation. Conclusions drawn from the work completed and recommendations concerning particle tracking with MODFLOW-VKD are made in Section 5.

1.5 Acknowledgements

This work has been completed with help from Sarah Evers and Paul Hulme of the Environment Agency's Ecosystems Science Group.

2 Steady State Particle Tracking

2.1 Introduction

This section covers Tasks 1 and 2 from the scope of work and concerns particle tracking at steady state. Task 1 involves the writing of a small FORTRAN program to extract cell-by-cell flows for individual timesteps from large time variant data sets. Task 2 is the setting up of steady state models for low and high groundwater conditions, particle tracking with the models and evaluation of whether this may be a practical aid to protection zone delineation with time variant Regional models.

2.2 Task 1: Extracting cell-by-cell flows

A small FORTRAN utility was developed that extracts cell-by-cell flows for individual timesteps from larger time variant cell-by-cell output files. The utility is written to work with binary output files produced by MODFLOW-VKD.

The program requires as input a small control file containing the following information:

1) The number of rows, columns and layers in the MODFLOW-VKD model.
2) A common element to be included in the names of the output files.
3) The number of timesteps to be extracted.
4) A list of the stress periods and timesteps to extract.

The user is prompted for the name of the time-variant cell-by-cell flows file. The output from the program is a number of individual cell-by-cell flow files, one for each timestep extracted. The format of the files is the same binary format written by MODFLOW-VKD.

As is explained in Section 2.4, it was eventually determined that whilst this utility program works as designed, the extracted cell-by-cell files can not be used for steady state particle tracking.

2.3 Particle tracking in Chalk aquifers and porosity values

Particle tracking requires the calculation of average linear velocity of flow through an aquifer, rather than the Darcy velocity (or specific discharge). This requires the user to enter values of the aquifer porosity. Since porosity is not require for standard water resource evaluations, and has not previously been entered for the Bourne and Nine Mile model used in this study, some consideration is given to the value of porosity to be used.

The Chalk is a dual-porosity aquifer, with the pores present in the rock matrix providing the main component of storage, and fissures the main component of permeability. The fracture system of the Chalk can be divided into primary and secondary fissures (Price 1987). The origin of the primary fissures is tectonic with typically 3 sets of fissures, 1 set parallel to the bedding plane and the other approximately perpendicular to it, and to each other. The secondary fissures are enlarged primary fissures as a result of processes including dissolution, stress release due to overburden removal and weathering.

The porosity of the Chalk matrix is typically in the order of 20-45% (Downing *et al*, 1993). However, the majority of the water present in pores is essentially immobile. As such advective transport processes do not affect pore water. The water in primary and secondary fractures is subject to advective processes. Chalk pores and the water contained in pores do partake in matrix diffusion and adsorption processes.

For the purposes of the present work, where the limitations of the continuous porous media assumption are recognised, it is necessary to define a realistic porosity for the Chalk that reflects relatively rapid transport processes. This means ignoring the high porosity of the Chalk matrix and representing the effective porosity of the primary and secondary fractures that contribute the majority of the permeability of the aquifer. In this case the porosity used for particle tracking will be the same as the unconfined storage (specific yield) of the aquifer (Price 2004).

The porosity values used in the particle tracking are therefore the specific yield values used in the time variant modelling of the Bourne and Nine Mile catchments. These are 0.01 for the majority of the Chalk outcrop and 0.005 for unit previously classified as Lower Chalk.

2.4 Task 2: Steady state particle tracking

Task 2 is steady state particle tracking at high and low groundwater conditions for the Bourne and Nine Mile model. The original intention was to use the cell-by-cell flows extracted the time variant Bourne and Nine Mile model and porosity values defined in Section 2.3. This was attempted with a steady state model set up in Groundwater Vistas using extracted time-variant output. It quickly became apparent that this technique is not possible due to the presence of the storage term in the cell-by-cell flows. This was not anticipated during the writing of the scope of work, although it is an obvious aspect of time variant simulations.

A solution to the storage issue with steady state models is to apply the time instant steady state approach.

2.5 Time Instant Steady State (TISS)

The TISS technique enables a steady state solution to the Regional flow equations to be produced for any snapshot in time. Rushton (2003) provides a brief description of the technique and examples of its practical application.

TISS involves forcing the model heads to a true steady state solution by altering the recharge to the aquifer. The technique can be explained by considering the time variant Regional groundwater flow equation in 2 dimensions:

$$\frac{\partial}{\partial x}T_x\frac{\partial h}{\partial x} + \frac{\partial}{\partial y}T_y\frac{\partial h}{\partial y} = S_y\frac{\partial h}{\partial t} - q$$

In order to force steady state, the first term on the right hand side of Equation 2.1 involving storage needs to be zero. In practice the way to do this is use an equivalent recharge, Re, to subtract the storage term.

$$R_e = q - S_y\frac{\partial h}{\partial t}$$

Equation 2.2

The flow equation then becomes:

$$\frac{\partial}{\partial x}T_x\frac{\partial h}{\partial x}+\frac{\partial}{\partial y}T_y\frac{\partial h}{\partial y}=-R_e$$

Equation 2.3

This numerical slight of hand can be illustrated with an example. If water levels are rising during a period of recharge, then water is being taken into storage. The rise in head indicates that more water is entering a unit cube of aquifer than can leave it under current hydraulic gradients. In order to prevent heads rising and to force steady state, the recharge is reduced by an amount equal to the change in storage. With this equivalent recharge applied, outflows equal inflows, heads remain constant and steady state is achieved.

Conversely, when groundwater levels are falling, water is released from storage and the change in storage is negative. To obtain steady state in this case, a negative storage contribution is subtracted from the recharge (equivalent to adding), resulting in an equivalent recharge greater than the actual recharge.

2.6 TISS for the Bourne model

Two TISS models were created for the Bourne and Nine Mile model corresponding to the highest and lowest groundwater conditions during the 30-year simulation. These occurred in February 1995 and October 1997 respectively. In the time variant model the high and low conditions occurred with Stress Periods 920 and 1014. The TISS models are based on these two stress periods of the time variant simulation.

The first step in creating a TISS model is the calculation of effective recharge. This consists of the following steps:

1) Re-run the time variant Bourne and Nine Mile model to save all outputs for the timesteps within the high and low conditions stress periods. This enables the most accurate calculation of changes in aquifer storage.
2) Calculate the change in head from the penultimate to the last timestep.
3) Calculate the flux of water taken into or out of storage by multiplying the head change by the aquifer's specific yield.
4) Convert the storage flux (m3/d) to a distributed recharge (m/d) by dividing by the cell area (250 x 250 m).
5) Calculate the equivalent recharge by subtracting the storage flux from the actual recharge for the stress period.

The first part of these calculations was completed within Groundwater Vistas (GWV) using the matrix array calculator. The final calculation of equivalent recharge was completed in an Excel spreadsheet and the results exported back to the user interface. The TISS recharge files were then written with GWV.

Other steps necessary to run the TISS models were:

- Exporting of boundary condition information for the respective stress periods and the creation of steady state boundary condition files. The boundary condition files created were:

- Wells files with abstraction information.
- Streams file with stream locations and associated parameters. This also includes discharges to surface watercourses.
- Drains file used in the Bourne and Nine Mile model to represent flow to the aquifer from PWS leakage and soak-away discharges to ground.
- Rivers file used to represent leakage from the Kennet and Avon canal crossing the northern portion of the model.

- Creation of standard MODFLOW files, the basic file, output control and PCG2 solver.
- Creation of a block-centred flow file. This file was set up such that the VKD function was **inactive.** The hydraulic conductivity array entered was calculated from the VKD transmissivity distribution and saturated depth. This method was used to simplify '.bcf' file creation.
- To run the resulting models to steady state using MODFLOW-VKD. It is necessary to use the VKD version of MODFLOW for the streams to function correctly (due to VKD changes in segment numbering and discharges).

Once the models had successfully run the steady state solutions were carefully compared with outputs from the time variant model at the appropriate stress periods. Differences in heads of less than 10^{-4} m were observed indicating that the TISS simulations functioned correctly.

2.7 Particle tracking in steady state

With the TISS solutions for high and low groundwater conditions completed, MODPATH was applied for particle tracking simulations.

MODPATH (Pollock, 1994) is a particle tracking post-processing package that was developed by the USGS to compute three-dimensional flow paths using output from MODFLOW, the USGS finite difference groundwater flow model. MODPATH uses a semi-analytical particle tracking scheme that allows an analytical expression of the particle's flow path to be obtained within each model cell. Particle paths are computed by tracking the particle from one cell to the next until it reaches a boundary or internal source/sink.

There are a number of limitations associated with MODPATH that should be highlighted, these relate to:

1) Underlying assumptions in the particle tracking scheme; the assumption that flow follows a simple linear velocity interpolation.
2) Discretisation effects are caused as a result of model cell size. Use of too large a cell size can cause problems such as weak sinks and lessen the accuracy of the velocity interpolation.
3) Uncertainty related the underlying groundwater flow model that is an approximation of the aquifer. The accuracy of particle tracks obviously depends on the accuracy of the flow model.

MODPATH simulations were run for the TISS models described in Section 2.6.

Two sites were chosen for particle tracking, the abstraction wells at Tidworth Garrison and Clarendon. Tidworth is a valley site close to the winterbourne section of the River Bourne. Transmissivity variations are at their greatest in this part of the Bourne and Nine Mile model where VKD is active. Clarendon is representative of an interfluve site located between the Rivers Bourne and Dunn in the southern part of the model. Whilst VKD is also active in this area, the transmissivity variations are significantly less than at Tidworth.

Table 2.1 presents model transmissivity values for these two sites under high and low groundwater conditions.

Table 2.1 Modelled heads and transmissivities at chosen sites

Location	Modelled value	High groundwater conditions	Low groundwater conditions
Tidworth	Head, m	109.00	82.03
	Transmissivity, m^2/d	3916.20	1374.20
Clarendon	Head	61.71	41.93
	Transmissivity, m2/d	1139.00	679.40

Backward particle tracking was applied in order to define capture zones contributing to the abstractions wells. Forty particles were released from each well. As the model is steady state there is no requirement to give a start and end date for tracking the particles.

Initially the particles were centred on the actual grid reference of the abstraction but there were spatial problems with this approach as particles tended to leave the cell from one side. Since in MODFLOW abstraction is effectively from the whole model cell, the particles were moved to surround the centre point in the cell. This resulted in a more radial pattern of initial particle traces as would be anticipated around a pumped well.

This issue highlights the grid size issue with MODPATH. Refining the grid would improve the accuracy of tracks, as the actual location of the well would be more closely represented. In the case of the Bourne model, the finite difference grid has not been refined further for particle tracking and it is acknowledged that the 250 x 250m mesh may be too coarse to provide accurate results.

2.8 Results of particle tracking

Figures 2.1 to 2.3 show the results of the TISS backwards tracking simulations for Tidworth and Clarendon for high and low groundwater conditions.

There is an obvious difference in the particle traces for high and low groundwater simulations. The capture zones for the high groundwater simulation are narrow, showing flow along very specific pathways. As the water table is at a maximum, transmissivities are at their highest, flows will be rapid, and only a small area is needed to support the abstraction. The higher velocity at high groundwater elevations is illustrated by the longer 50 and 400-day travel zones.

In contrast, the capture zone for the abstractions during low groundwater levels is much larger, reflecting the lower recharge. With low groundwater levels the aquifer transmissivity is also reduced. These two factors reduce the particle’s velocities leading to shortened 50 and 400-day travel zones. With low groundwater levels the winterbourne section of the River Bourne is dry and particles from Clarendon move under the bed of the river.

2.9 Discussion

The two TISS models represent the extreme cases of possible catchments for the abstraction wells. In each case it is assumed that the most extreme conditions between 1970 and 1999 (the period of the Bourne model simulation) will be constant for an infinite length of time. Whilst particle tracks of the TISS models permit the remotest possibilities to be examined these conditions can never occur in reality due to the large seasonal variation in recharge and consequent head changes.

Historical observations show that the system is highly dynamic with significant seasonal changes in recharge, groundwater levels and streamflows. These constantly variable conditions cause aquifer flow rates and directions to change and particle speeds and directions to vary throughout the year.

More realistic capture zones for the abstractions are likely to be a mixture of the two extremes. The current SPZs for Tidworth and Clarendon (Figure 2.4) are closer in appearance to the low groundwater table TISS simulation. The SPZ for Clarendon is extremely wide and the total capture zone tail extending up the catchment has been truncated. The SPZ for Tidworth is merged into the SPZ for Bulford but is similar in appearance to the low groundwater simulation. There is no difference between the 400-day travel zone and total capture zone. These SPZs probably result from steady state models using Flowpath completed in the mid-1990s.

The primary objective of the steady state models and particle tracking was to test the steady state methodology as a route by which the Agency's Regional groundwater models could be used for SPZ delineation. The TISS particle tracking demonstrates that:

- For high and low conditions groundwater conditions only the absolute extremes of particle tracks and SPZs results.
- The particle tracks for steady state extreme conditions are significantly different.
- Neither of the extremes are probably of much help for the revision of SPZs.

It is concluded that the steady state methodology, using extremes of high and low groundwater elevations, is not a viable method for revising SPZs using Regional models. The case of average groundwater conditions was not considered during the present study. This could be helpful, but would still not make full use of the time variant nature of Regional models.

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Figure 2.1 Time instant steady state backwards tracking for high and low groundwater levels

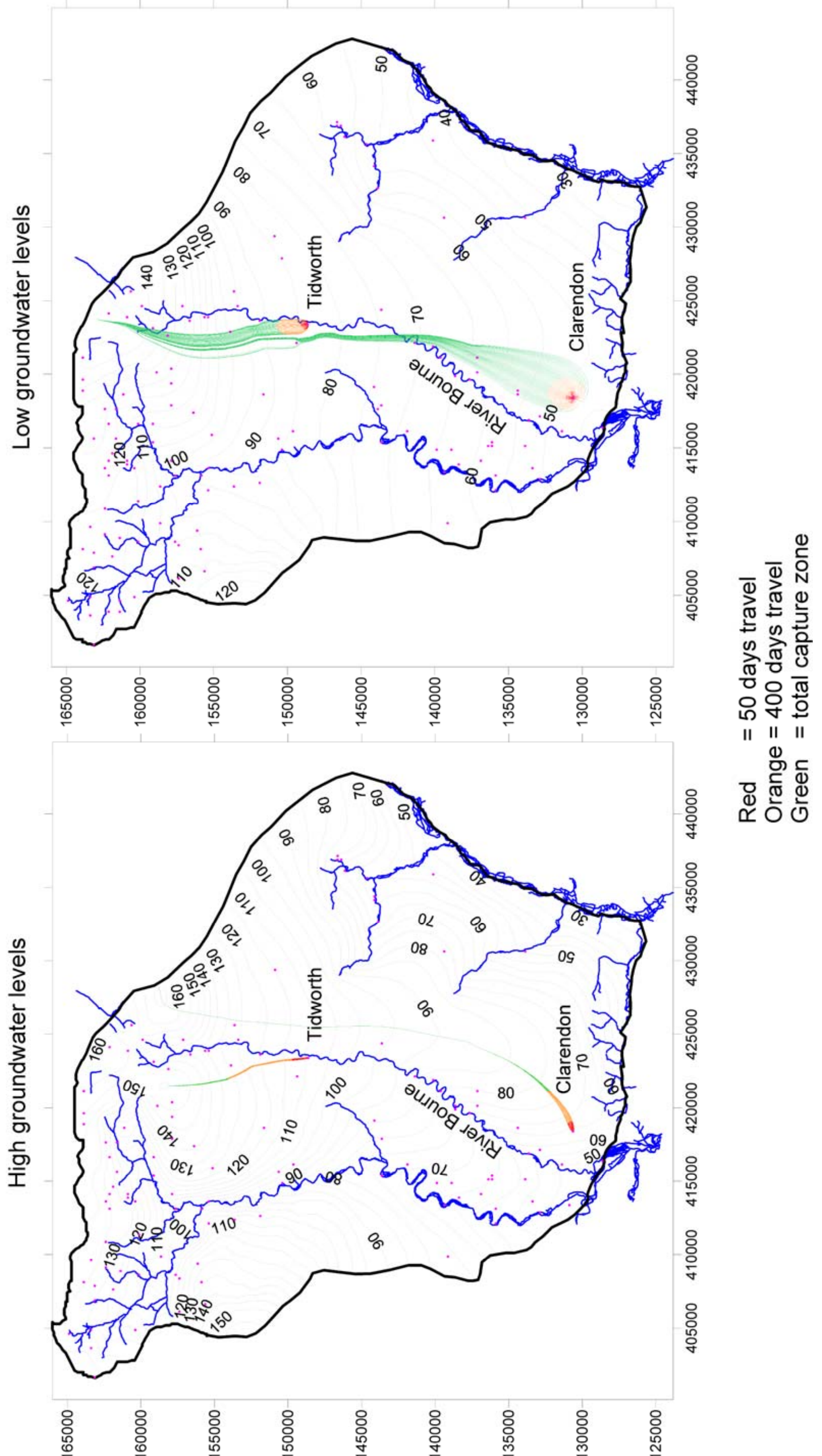

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Figure 2.2 Time instant steady state backwards tracking from Tidworth abstraction

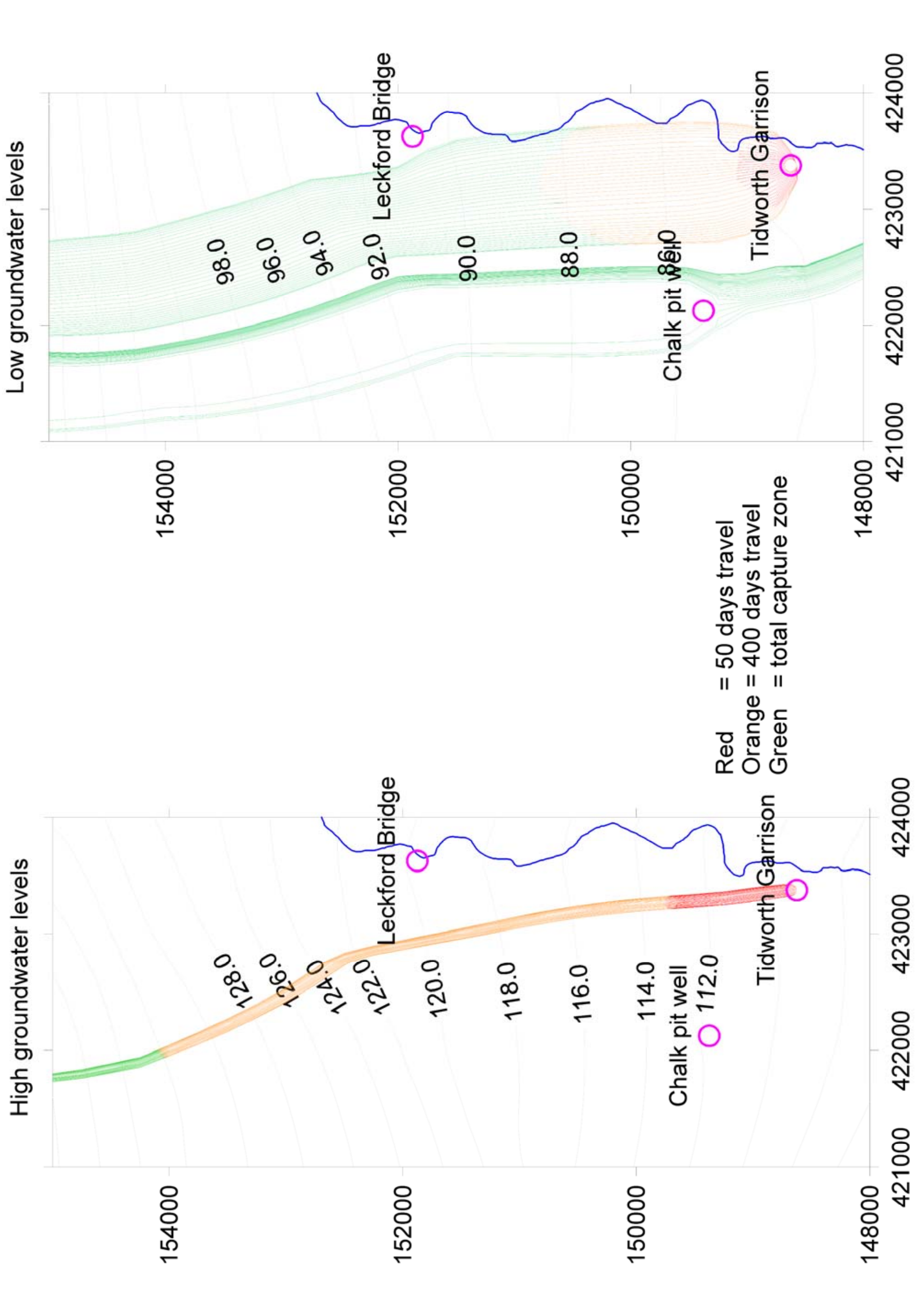

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Figure 2.3 Time instant steady state backwards tracking from Clarendon Park abstraction

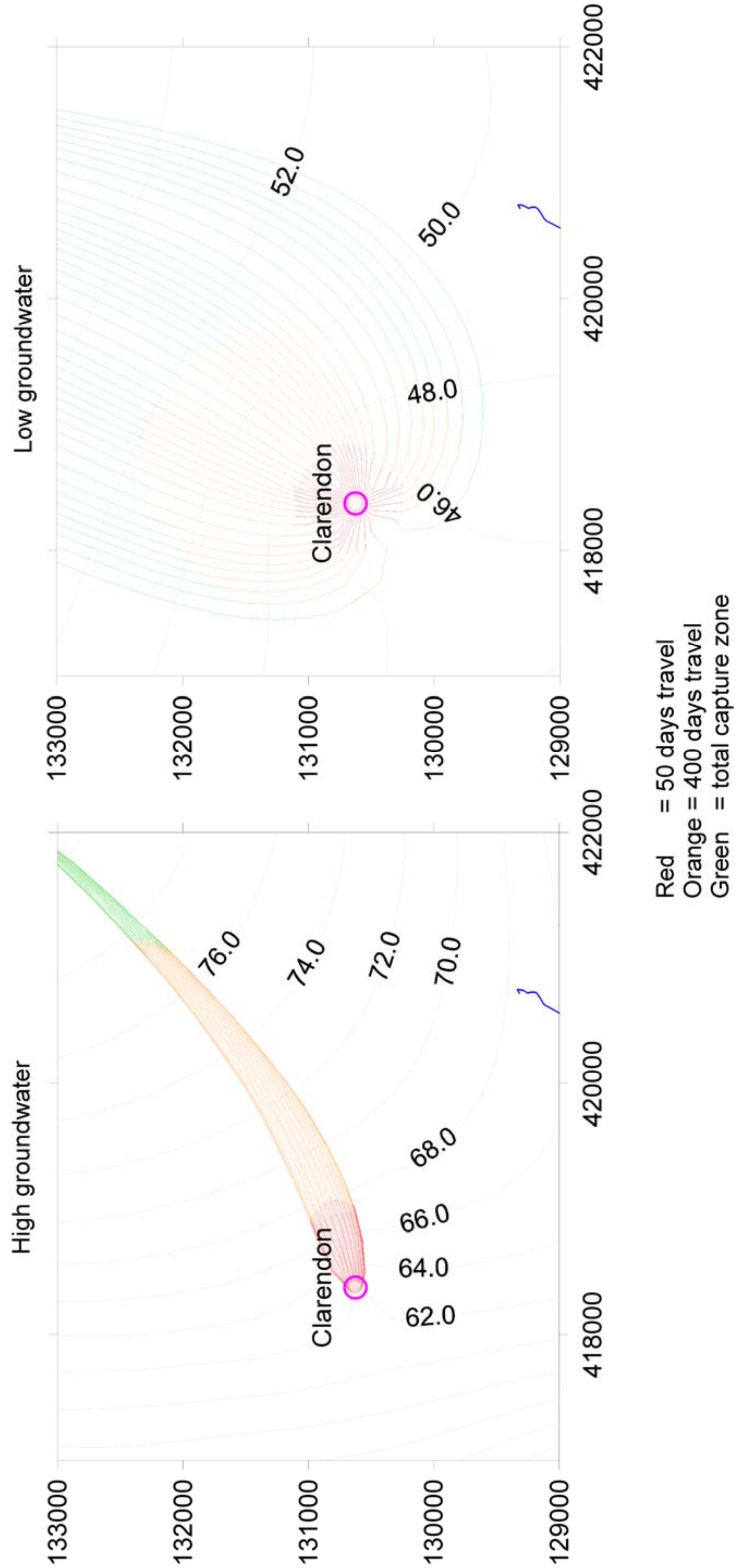

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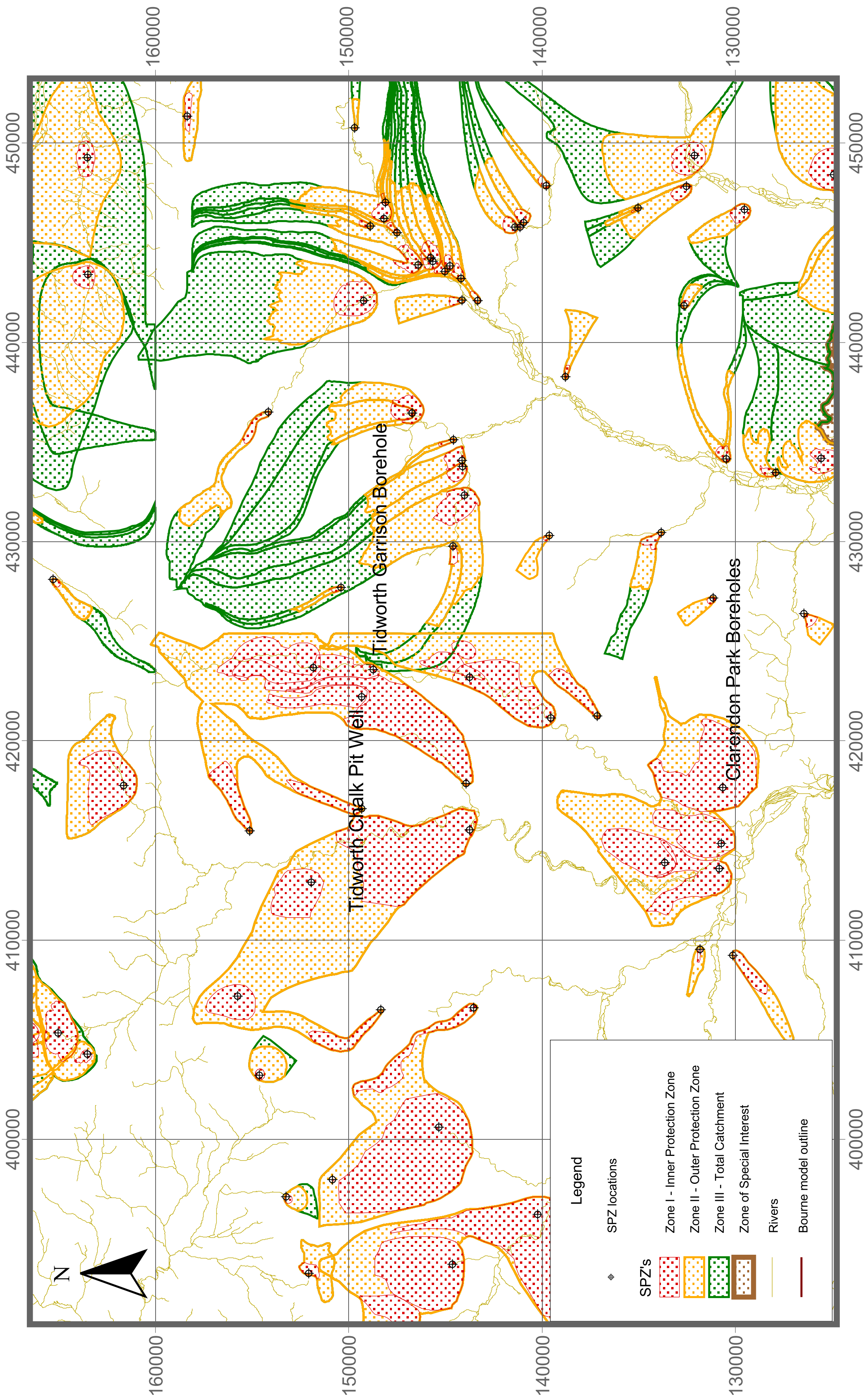
Figure 2.4 Existing source protection zones



3 Effects of VKD on Particle tracks

3.1 Introduction

Task 3 of the scope of work concerns adapting the particle tracking algorithms to take account of VKD. The adaptation used was developed for the ZOOMQ3D model, a 3-dimensional object-orientated groundwater model developed jointly by the Environment Agency, BGS and Birmingham University. This section describes the testing of the adaptation with MODPATH and examines the effect that VKD has on particle tracks.

MODFLOW VKD is a modified version of the USGS MODFLOW-96 groundwater modelling code (Harbaugh & McDonald, 1996). The main focus of the modifications to MODFLOW is the inclusion of variation of hydraulic conductivity and storage with depth to represent parameter changes in the zone of fluctuation in chalk and limestone aquifers.

The modification to MODFLOW allows the hydraulic conductivity to vary with depth within a single model layer. This gives a non-linear relationship between transmissivity and groundwater level, improving the representation of field conditions. The underlying issues and implications of the changes introduced in MODFLOW are detailed in the Project Report NC/00/23 - *Enhancements to MODFLOW, user guide for MODFLOW-VKD* – a modified version of MODFLOW-96 to include variations in hydraulic conductivity with depth (Environment Agency, 2003).

Before making adaptations to take account of VKD, consideration is given to what happens if MODPATH is applied, without any modification, to a VKD model.

3.2 Using MODPATH with VKD models

Application of VKD implies differences in groundwater velocity at different elevations within a model cell. At low groundwater conditions, if below the VKD inflection point, the velocity field in each cell is uniform with elevation and is proportional to the base hydraulic conductivity, Kbase. At high groundwater elevations the velocity field close to the water table will be greater than that below the VKD inflection point. With the velocity field varying with elevation within a cell, and with time as groundwater levels fluctuate, the time and elevation of particle release become key factors influencing particle velocity.

MODPATH assumes that within a model cell there is a uniform flow through the cell at all elevations. In the x-direction flow is signified by the equation (Freeze and Cherry 1979):

$$Q_x = V_x . \eta . A$$

Equation 3.1

Where:

Q_x is the flux in the x-direction

V_x is the average linear velocity in the x-direction (not the Darcy velocity)

η is the porosity

A is the cross sectional area of the cell.

Therefore the average linear flow velocity in the x-direction is:

$$V_x = \frac{Q_x}{\eta A}$$

Equation 3.2

MODPATH was developed to work with “normal”, non-VKD, MODFLOW where aquifer properties are constant within model cells. MODPATH is therefore based on the reasonable assumption that X, Y and Z velocity components are uniform over the cell faces for which they are calculated, i.e. Vx, is the same at Zb, the cell base, as at ZT, the cell top.

When MODPATH calculates the velocities across a cell it uses the cell-by-cell flows written by the MODFLOW simulation and a form of Equation 3.2. MODPATH does not require the cell’s hydraulic conductivity for this calculation – only flows.

Taking the case of high groundwater levels in a VKD simulation, the flux through a cell will be greater than a non-VKD simulation as more water is able to move through the cell at high elevations, as illustrated in Figure 3.1. The cell-by-cell flow file written by a MODFLOW-VKD simulation has this larger flux recorded in it. MODPATH reads the flow and uses a form of Equation 3.2 to calculate the X-direction velocity component for that cell face. Since MODPATH assumes that velocity components are uniform over a cell face, the resultant Vx calculated is a depth averaged velocity. The high velocity at the top of the VKD profile and the lower velocity below the inflection point are smoothed to a single mean velocity for the cell face.

Through a time-variant simulation, as groundwater levels vary seasonally, the depth averaged velocity will vary, reflecting changing flow rates and the presence of VKD. This is an important point - particle tracking performed by MODPATH on a VKD simulation actually takes VKD into account, to some extent, by using a depth-averaged velocity.

3.3 Particle tracking taking account of VKD with ZOOPT

It is possible to take fuller account of the effect of VKD on particle velocities. The ZOOMQ3D code does this, varying the velocity of particles with their elevation within the cell.

ZOOMQ3D incorporates particle tracking with the ZOOPT program, which takes account of cells where VKD is active. The ZOOPT approach applies a factor to the velocity calculation that takes account of the hydraulic conductivity (K) at the elevation of the particle compared to the vertically averaged K.

3.3.1 ZOOPT approach

This description of the ZOOPT approach is taken from the ZOOMQ3D manual, (Jackson *et al*, 2004).

The pathlines of particles under advection alone are governed by the equation:

$$\frac{\partial p}{\partial t} = v(p,t)$$

Equation 3.3

where:

p = x **i** + y **j** + z **k** is the position vector
v = v_x **i** + v_y **j** + v_z **k** is the seepage velocity vector
$v_x = \frac{K_x}{\theta}\frac{\partial h}{\partial x}$
K_x is the hydraulic conductivity in the x-direction
θ is the porosity and,
h(x,y,z,t) is the groundwater head, which is a function of space and time

The solution of Equation 3.3 for the position of a particle at time, t, is:

$$p(t) = p(t_0) + \int_{t_0}^{1} v(p,t)dt$$

Equation 3.4

where:

$p(t_0)$ is the initial position of the particle at time t_0.

In cells where hydraulic conductivity varies with elevation the Runge-Kutta particle tracking technique must be used to define the path lines. The integral in Equation 3.4 cannot be evaluated analytically because the horizontal velocity varies in the z-direction, that is, towards the top of the VKD profile the horizontal velocity is greater than towards its base. Within ZOOPT the assumption is made that the horizontal velocity of the particle is proportional to the horizontal hydraulic conductivity at its location. The component of the velocity in the x-direction at the cell walls at x_1 and x_2 are given by:

$$V_{x1}(z) = \frac{K_x(z)}{\overline{K_x}}.\frac{Q_{x1}}{\theta \Delta y(z_2 - z_1)}$$
$$V_{x2}(z) = \frac{K_x(z)}{\overline{K_x}}.\frac{Q_{x2}}{\theta \Delta y(z_2 - z_1)}$$

Equation 3.5

where:

$V_{x1}(z)$ and $V_{x2}(z)$ are the x-components of velocity (m day^{-1}) on the cell walls at elevation z,

Q_{x1} and Q_{x2} are the flow rates entering and exiting the cell in the x-direction (m^3 day^{-1}),

$K_x(z)$ is the hydraulic conductivity (m day^{-1}) in the x-direction at elevation z,

$\overline{K_x} = \frac{1}{(z_2 - z_1)_{z1}} \int_{z_1}^{z_2} K_x(z)dZ$ is the mean hydraulic conductivity (mday^{-1}) in the x-direction,

θ is the porosity of the node,
Δy is the width of the node in the y-direction (m) and,
z_1 and z_2 are the elevations of the bottom and top of the node (m).

3.4 Implementation with MODPATH for Bourne TISS models

The algorithm used in MODPATH to calculate the velocity field across the cell is based on linear interpolation based on flows though each model cell face. The implicit assumption that the velocity field is linear through the cell does not hold for VKD, at elevations above the inflection point the velocity should vary.

To see the effect of VKD on MODPATH particle tracks for a MODFLOW-VKD model, the TISS simulations of the Bourne and Nine Mile River are used. For the application of factoring in MODPATH it is assumed that the model is in steady state. It is also assumed that the model is isotropic, as is the case with the Bourne model.

Two elevations of particle are considered:

- High elevation, at the water table and above the VKD inflection point for the high groundwater condition.
- Low elevation, below the inflection point for the low groundwater condition.

To see the effect of VKD on particle tracks in MODPATH the ZOOPT correction factor must be applied. Equation 3.5 above can be re-written as:

$$V_{x1}(z) = \theta' \frac{Q_{x1}}{\Delta y(z_2 - z_1)}$$

Equation 3.6

Where the parameter θ' is given by:

$$\theta' = \frac{K_x(z)}{\theta \overline{K_x}}$$

Equation 3.7

The parameter θ' is effectively a modified porosity value. At locations above the VKD inflection point where K_x is greater than $K_{(average)}$ the modified porosity θ' is greater than it would be were the water table below the inflection point. An increased modified porosity θ' causes an increase in particle velocity. Conversely when K_x is less than the depth average $K_{(average)}$, θ' is lower and the particle velocity decreases.

The modified porosity incorporates the VKD correction into a steady state MODPATH simulation by replacing the original porosity. This enables corrections for VKD without having to alter the MODPATH source code.

The parameter θ' is calculated in a spreadsheet for the high groundwater condition. The particle elevation is assumed to be at the water table, the top of the VKD profile. The corrected cell-by-cell porosity values are then placed into the main 'Modpath.dat' file before the simulation is run. Porosities are either lower than or equal to the original steady-state MODFLOW porosities. This results in particles moving more quickly through the simulation.

3.5 Results and discussion of VKD correction

3.5.1 Variation of transmissivity with time

Before considering the difference in particle tracks the variation introduced by VKD in the Bourne model is examined. Figure 3.2a presents plots of transmissivity through time at Shipton Bellinger, located approximately 2km south of Tidworth. Two transmissivity plots are shown, with and without VKD active. When VKD is inactive there is a seasonal transmissivity change of around 500 m2/d. With VKD active there is a much larger variation in transmissivity, with the seasonal range usually being at least double the range of the base case.

Figures 3.2b and 3.2c show how the VKD and non-VKD model transmissivity profiles compare statistically. The "transmissivity duration curve" shows that with VKD active, transmissivity is within 10% of the non- VKD value for 44% of the time. It is greater than the non-VKD case for 38% of the time and less than the non-VKD case for 62%.

The two TISS simulations fall at opposite ends of the transmissivity duration curves and represent extreme conditions for the aquifer.

3.5.2 Effect of correction on particle traces

Figures 3.3 and 3.5 show the results of particle tracking with the VKD correction. The shape and direction of the particle traces is unaltered for both simulations. The only changes seen are in the travel times. This is to be expected. Since the model is isotropic, the factoring in X and Y directions is equal, meaning that the magnitude of the velocity vector changes, but not its direction.

Figure 3.4 presents distance v time plots for individual particles released from Tidworth and Clarendon for:

1) High groundwater levels, no VKD correction.
2) High groundwater levels, with VKD correction.
3) Low groundwater levels, no VKD correction.
4) Low groundwater levels, with VKD correction.

Tidworth

There is a clear difference in the traces during high water table conditions. The parameter θ' is approximately 2 at Tidworth during high water table conditions and this is reflected in the doubling in length of the 50 day travel zone from approximately 1 km to 2 km. There is no change in the direction of particles.

At low groundwater levels the traces are essentially identical to the un-corrected simulation. There is therefore no difference in the 50-day and 400-day travel times.

Clarendon
The high groundwater elevation plots show the same trend as at Tidworth, with particles moving more quickly with the VKD correction.

At low groundwater levels there is a small difference between the non-VKD and VKD tracks. This is a reflection of the elevation of Vmid, the VKD inflection point, which at Clarendon is just below the low groundwater elevation. The difference is apparent in the 400 day low groundwater traces at Clarendon.

3.5.3 Conclusions from particle track correction

The following conclusions are drawn regarding correcting particle tracks for VKD:

- It is possible to correct particle tracks for the effects of VKD in steady state models without modifications to MODPATH.
- The ZOOPT correction technique as applied using factored porosity can only be done for steady state models and is only applicable to isotropic systems. The ZOOPT correction could be incorporated into MODPATH for use with time variant models, but this would require considerable work.
- In an isotropic, steady state, model VKD only affects the magnitude of the velocity vector, therefore the speed of particles increases but there is no change in particle direction.
- Particle speeds increase above the VKD inflection point and are at their maximum either above the Vmax elevation or at the water table.
- The 50-day and 400-day capture zones are typically larger for VKD corrected runs. The total capture zone remains the same.

The plots showing how transmissivity varies with time in the Bourne model highlight that the TISS models represent the most extreme aquifer conditions of the 30-year Bourne and Nine Mile model simulation. The particle track correction for VKD has been shown to be possible, but the usefulness of applying such a correction to TISS models of the most extreme conditions is doubtful. Greater validity could be given to particle tracks from a steady state simulation of average groundwater conditions. Given that Regional models simulate significant time period of 20-40 years, a time variant particle tracking methodology would be preferable.

Figure 3.1 Flow through cell boundaries with and without VKD present

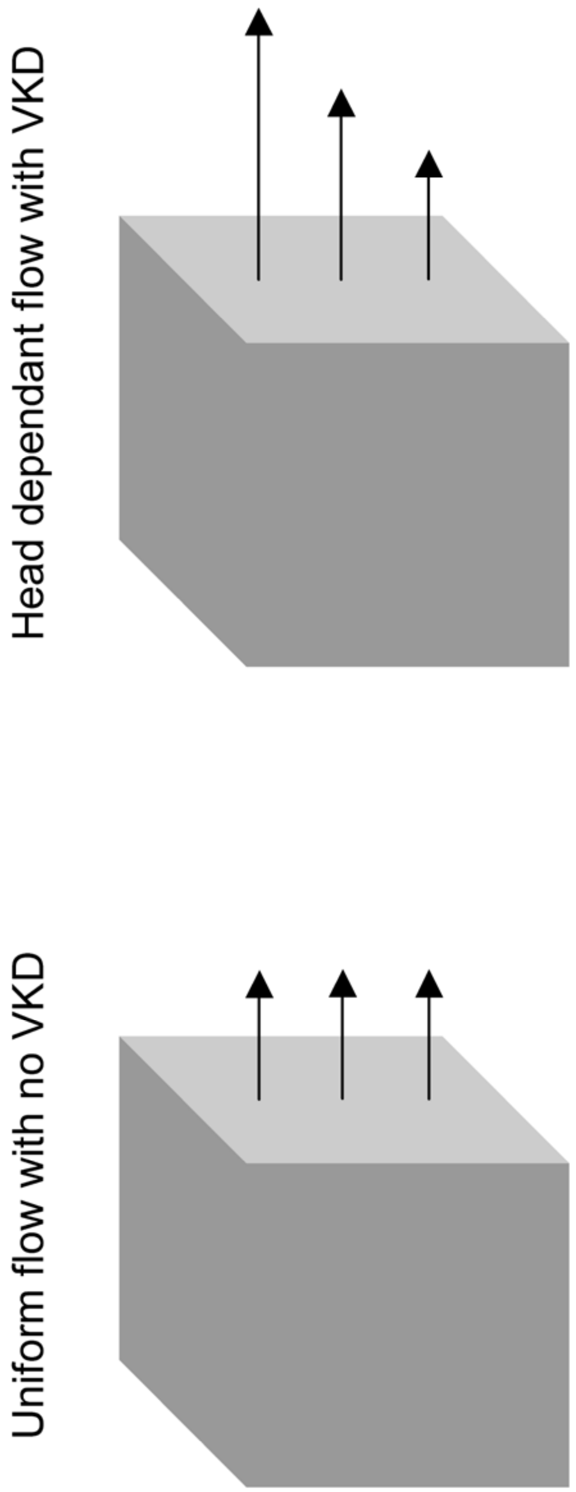


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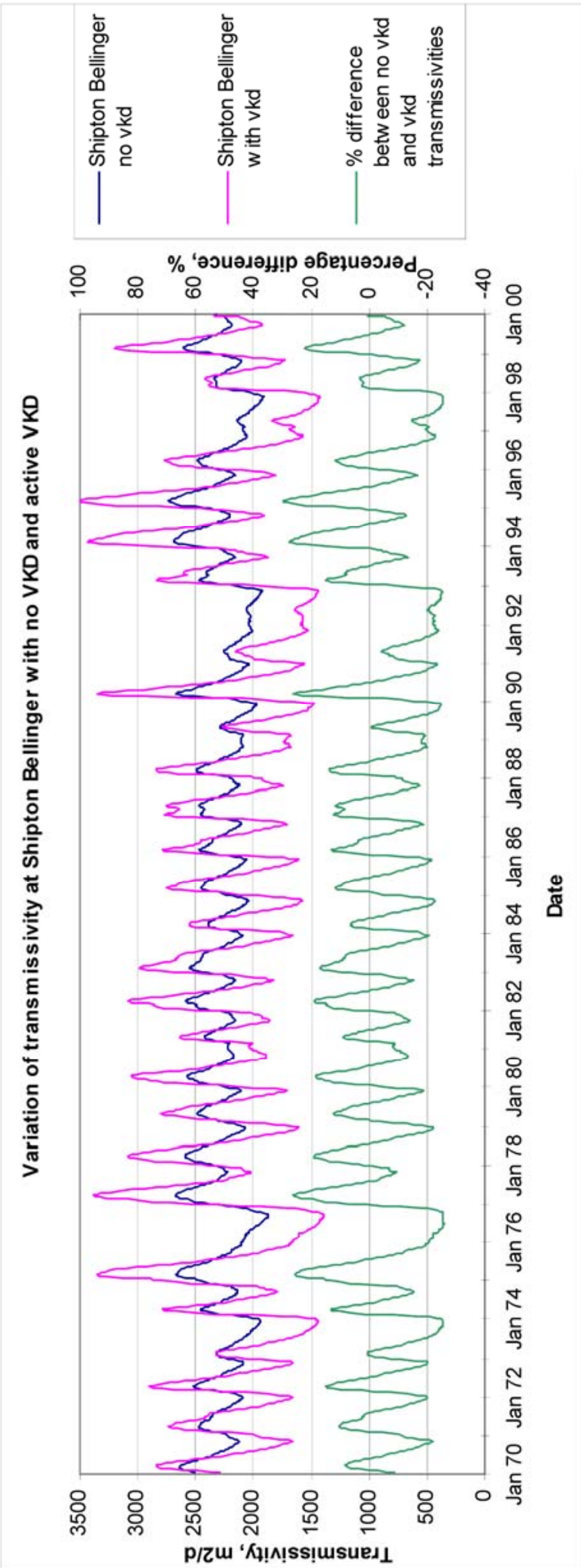
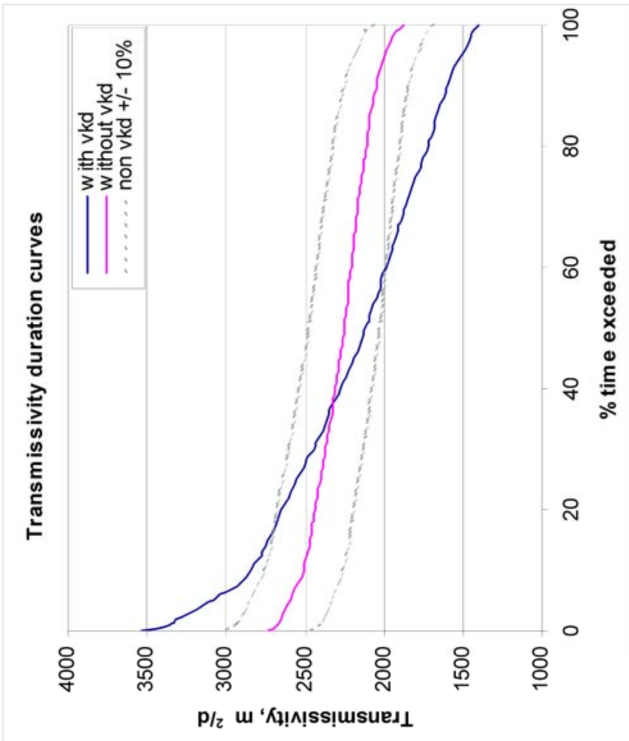
Figure 3.2 Transmissivity variation at Shipton Bellinger





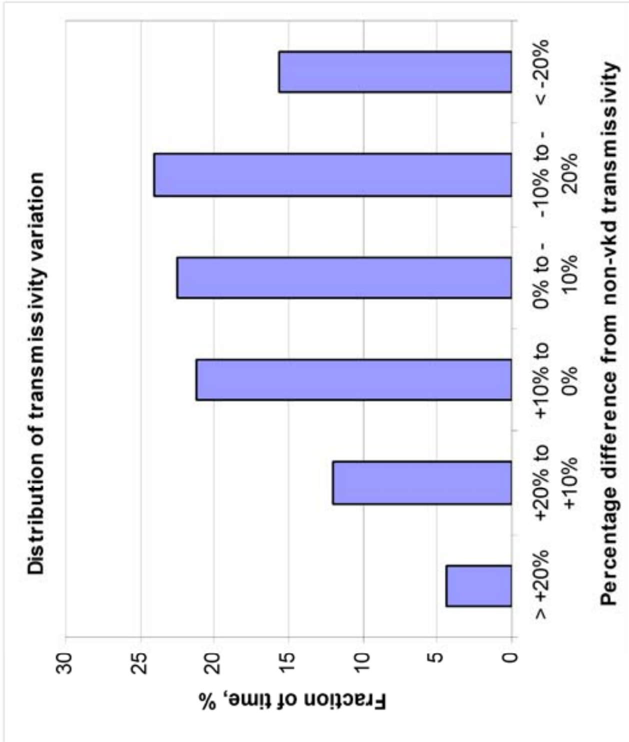


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Figure 3.3 Steady state backwards tracking from Tidworth abstraction with VKD correction

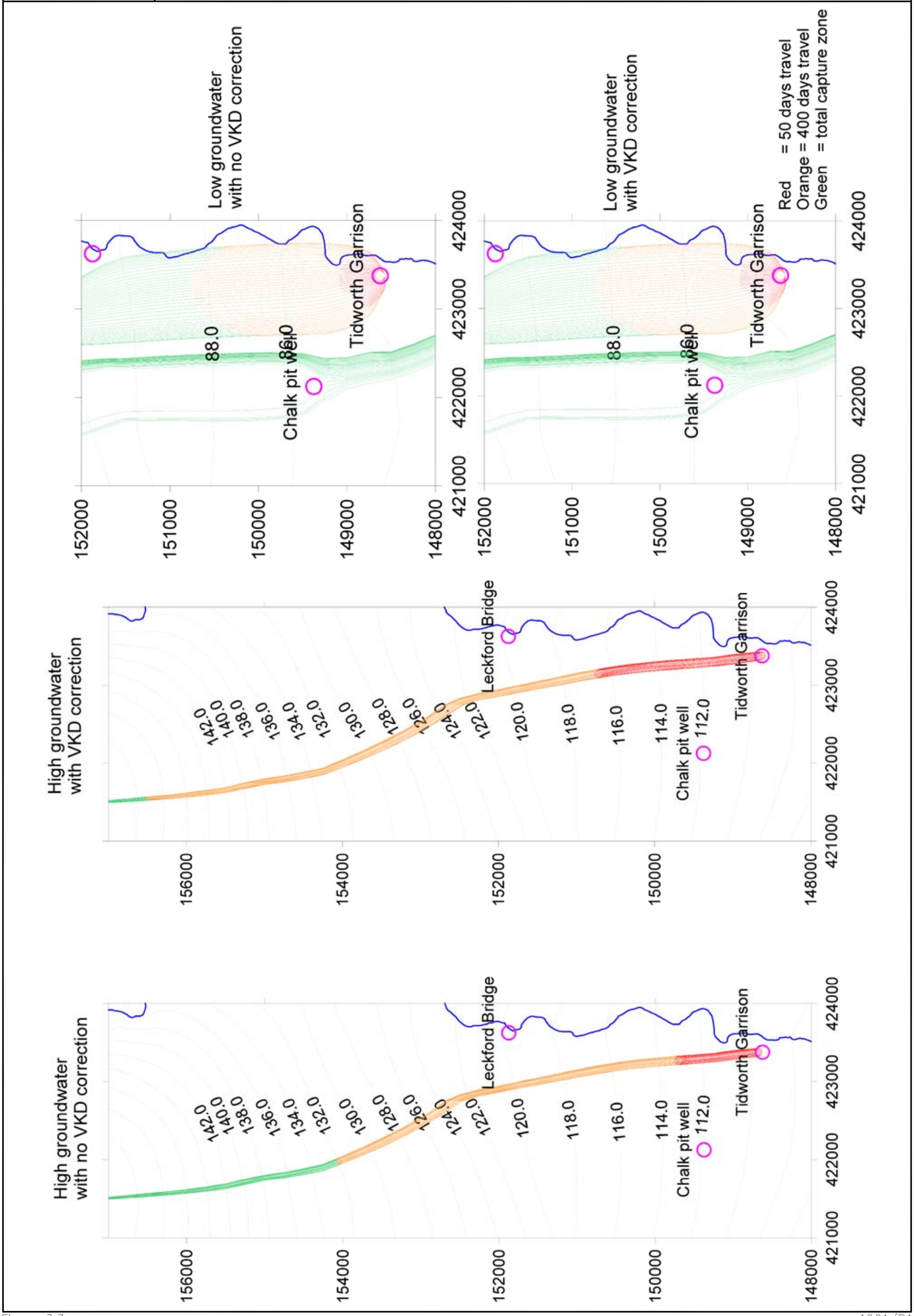

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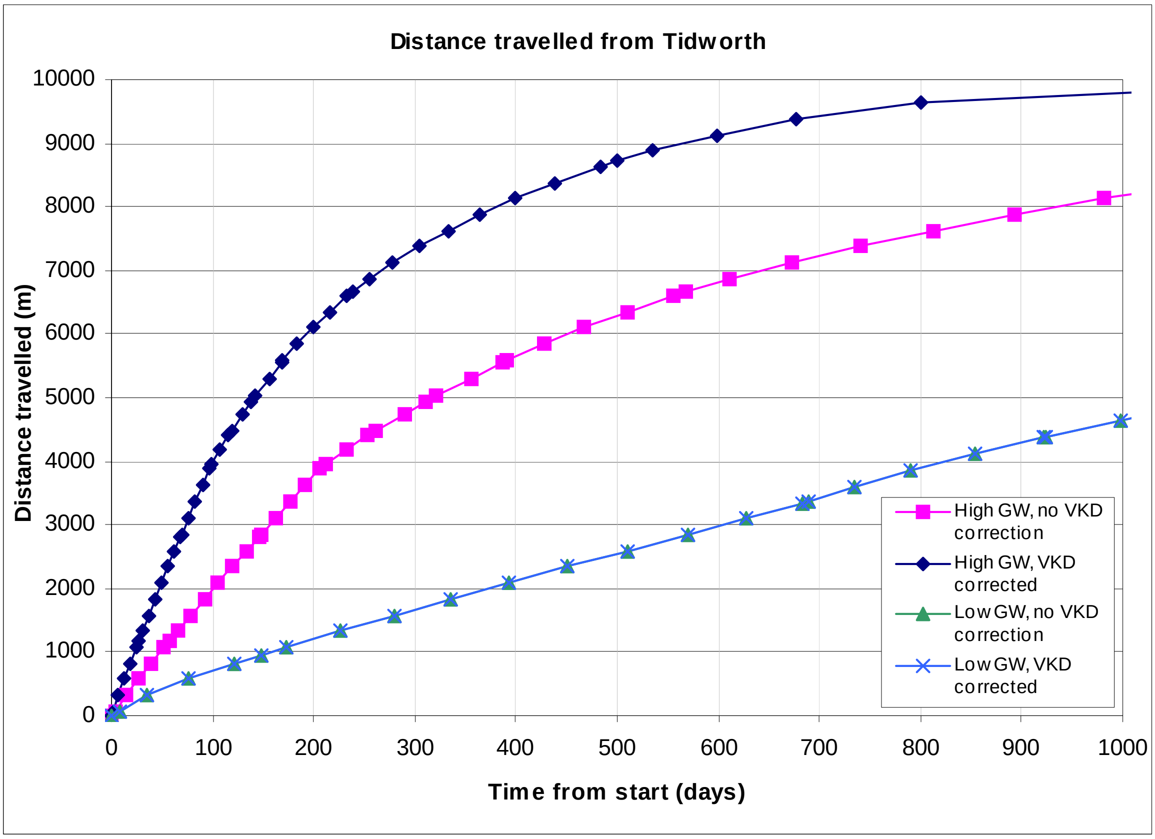
Figure 3.4 Individual particle traces through time from Tidworth and Clarendon



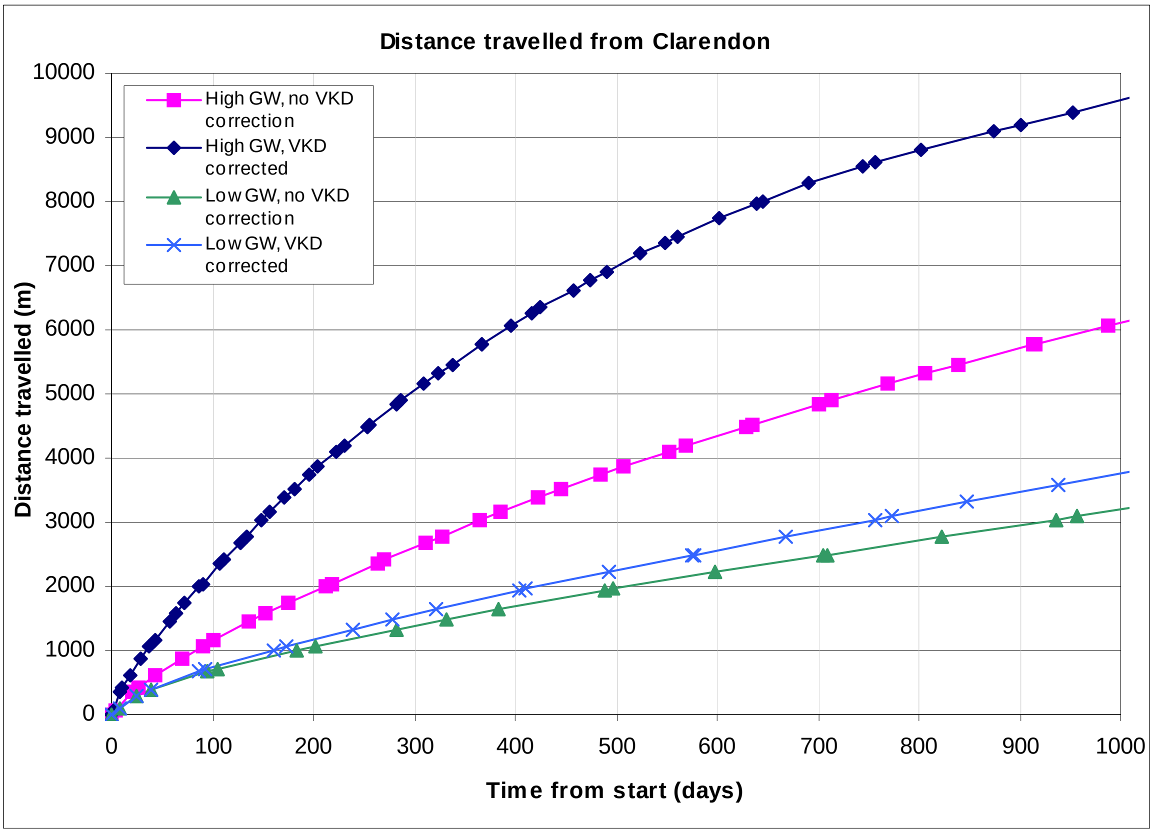


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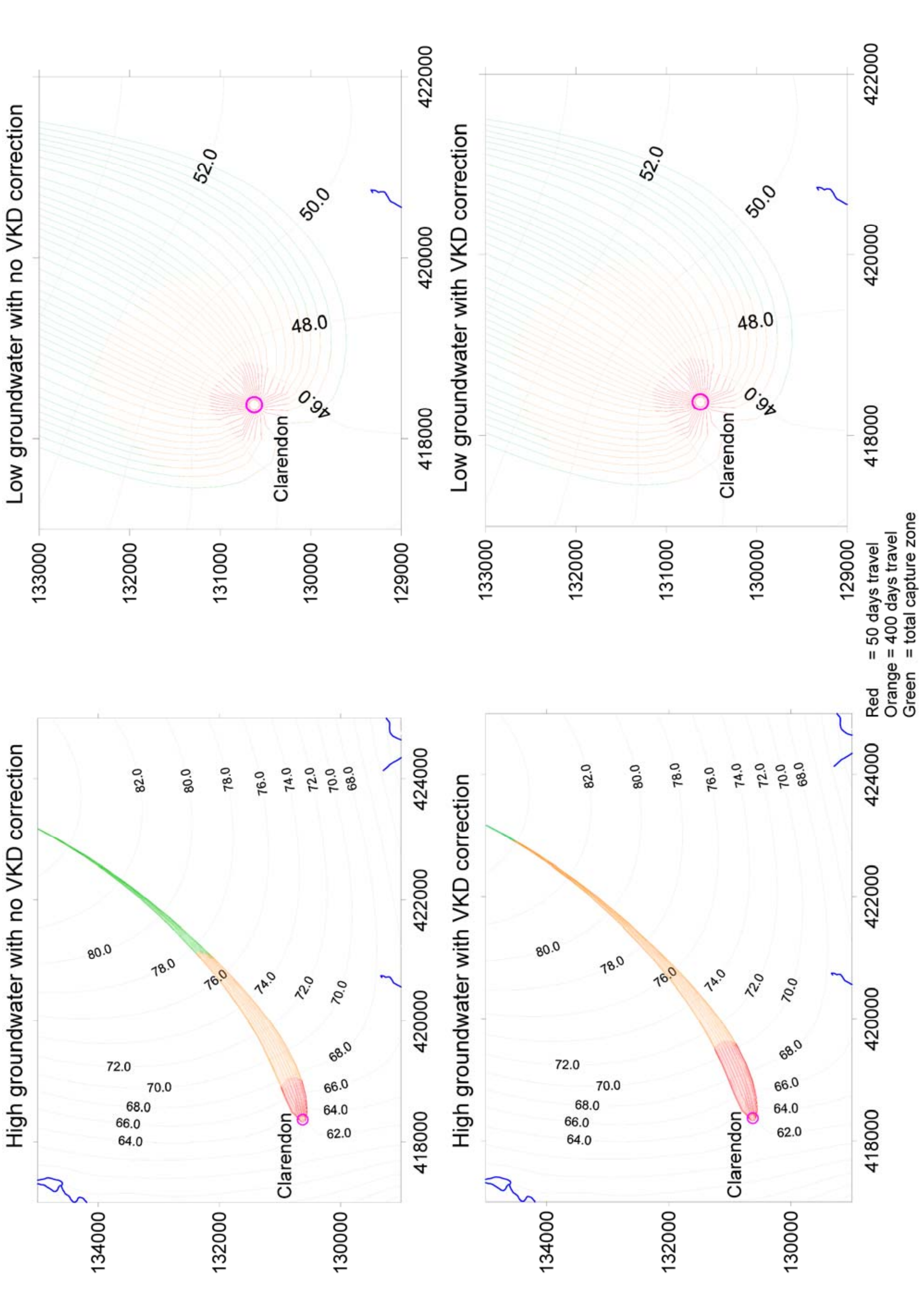
Figure 3.5 Steady state backwards tracking from Clarendon Park abstraction with VKD correction



4 Time variant particle tracking with Regional models

4.1 Introduction

In this section alternatives to steady state particle tracking for protection zone delineation are considered. The work in this section falls outside the original scope of work but is included since a potential methodology for time variant GPZ delineation was developed. As the work is out of scope, only limited investigation was possible.

Particle tracking can be performed in forward (down-gradient) and backward (up-gradient) modes. Consideration is given to the potential role of both of these tracking options for use with time variant models.

MODPATH treats transient simulations as a series of steady state flow periods. For each time step heads are considered constant and the same semi-analytical approach is used to calculate hydraulic gradients across model cells. At the end of the time step new heads and flows are read and the cell hydraulic gradients recalculated. Particles movement can be considered as a series of discrete jumps from one time step to the next.

Time variant particle tracking takes account of the constantly changing aquifer system, such as seasonal increases and decreases in recharge. There are still limitations to this approach, such as the accuracy of the underlying model, but the constraints and assumptions of the steady state method are mainly overcome. One potential issue concerns the time discretisation for transient simulations. If time steps used in rapidly changing conditions are too large then the accuracy of the particle tracking will be compromised. The issues regarding the grid spacing mentioned in Section 2 also still apply.

MODPATH 3.2, the latest version released for used with MODLFOW 96 format files was used for the forward and backward tracking. The Groundwater Vistas literature does not make it clear exactly which MODPATH version is compiled for use, but from its functionality it is Version 3.2.

4.2 Backwards tracking

Backwards tracking has the advantage that only particles released at a point of interest are tracked. As particles are released from the abstraction cell and tracked backwards they move to show the origin of water reaching that cell. If sufficient particles are released then all possible flow directions will be included. Along with determining the direction of travel the particles can be followed backwards through time. The 50-day and 400-day capture zones can easily be determined by mapping the spatial extent of the particles after each interval.

In terms of the MODPATH processing, backward tracking involves reading flow model output files up to the release time, keeping this data in memory, and then processing the particles backwards in time until they reach recharge sources. This is a complex process and MODPATH / GWV MODPATH can only process one release time per simulation. For example with the Bourne model, particles can be released around a pumped well on a set date, say 1st February 1995, and then tracked backwards in time to recharge in the preceding 0-3 years, in the case of a low storage system like the Chalk. To release particles at different times in the simulation, and hence cover all possible directions and distances, the model would have to be re-run for each start date. This limits the number of start dates possible due to the time constraints from setting up and processing each new MODPATH run. Due to this limitation, backwards tracking has not been pursued further, although automation of backwards tracking to cover multiple start times is theoretically possible.

4.3 Forward tracking

Forward tracking follows a particle forwards in time from a particular point. A grid of particles released and forward tracked can show the direction of groundwater flow through the grid area. One advantage of forwards tracking in MODPATH is the ability to include different release dates within in a single MODPATH run. This avoids repeating each simulation many times to get a representative capture zone resulting from releases at high and low groundwater levels.

The disadvantages of forward tracking are that large numbers of particles have to be released to reveal pathlines through the aquifer and to illustrate abstraction well capture zones. The definition of time-variant capture zones by considering the full paths of a grid of multi-time released, forward tracked particles, presents considerable data analysis problems. However, MODPATH includes in its output a subset of the particle tracking data called the endpoint file. This contains start and end locations of particles. The time-variant particle tracking methodology developed here uses a subset of data stored in the endpoint file.

4.3.1 Multiple particles, multiple release times

To illustrate the time-variant forward tracking idea a grid of particles is released at multiple times around the Tidworth abstraction considered in Sections 2 and 3. A large grid with a particle spacing of 50m by 50m is placed around the abstraction cell. The extent of the grid is based on the results of the TISS high and low groundwater simulations, which act as a guide to the extent of particle travel.

The grid is then copied so that particles are released for 74 stress periods starting in Jan 1994 and ending in Jan 1996. Once the particles have all been released tracking is continued for a further three years. This is to give time for particles to be captured by the pumped well. This approach leads to a large number of particles being tracked, e.g. in this example area of 2.75 by 7.75 km with 74 release times there are 646,000 particles. More particles would be required if the capture zone was expected to be larger and more release dates were required. Increasing particle spacing would reduce the number of particles required.

The MODPATH files are modified so that:

- The zone number for the Tidworth abstraction is given a unique number in the Ibound array in the main MODPATH data file. This ensures that the post processing is simpler as particles that end in this zone can be easily extracted for further analysis.

- All particles that enter the model cell containing the Tidworth abstraction are captured. This circumvents the weak sink problem with some particles continuing through abstraction cell if groundwater levels and flows are high or abstraction low.
- Only the endpoint file is written for the simulation. The endpoint file contains the spatial locations of each particle at the start and end of the simulation, along with the release date and date of termination of the particle if it is stopped during the simulation. It is not possible to continue writing the pathline file as its large size reaches the operating system file size limit.

4.3.2 Post processing and figure production

The endpoint file is processed using a FORTRAN program. The program reads the endpoint file and, for each particle release position, calculates the number of times released particles are captured at the pumped well. The program outputs a file containing particle locations and the number of capture times. This file can then be analysed and converted to a probability contour plot using a contouring package such as Surfer.

For the example, the number of particles released from each location is 74, equal to the number of release dates in the simulation. If a particular particle moves to the selected abstraction cell for all of the release dates, the program counts 74 captures and it is classed as a 100% capture probability. If the particle is only captured for 10% of the release times then the chance of the particle being captured is only 10%.

The file output by the FORTRAN program is contoured in Surfer to produce a figure showing the probability of particle capture, Figure 4.1. As would be expected the particles immediately upstream of the well were captured 100% of the time with particles further from the pumped well captured less frequently.

In this example only 74 out of 1096 stress periods are considered. Analysis of data file sizes shows that file size limits will not be exceeded if the whole 1096 stress periods were considered.

4.4 Discussion and conclusions

The time variant capture zone approach offers a way to apply time variant Regional models to groundwater protection zone delineation. The advantages of the technique are:

- Full account is taken of the seasonal variations in recharge, heads and velocities within the aquifer.
- The resultant capture zones include a degree of uncertainty analysis.
- The technique is equally applicable to aquifers other than the Chalk.

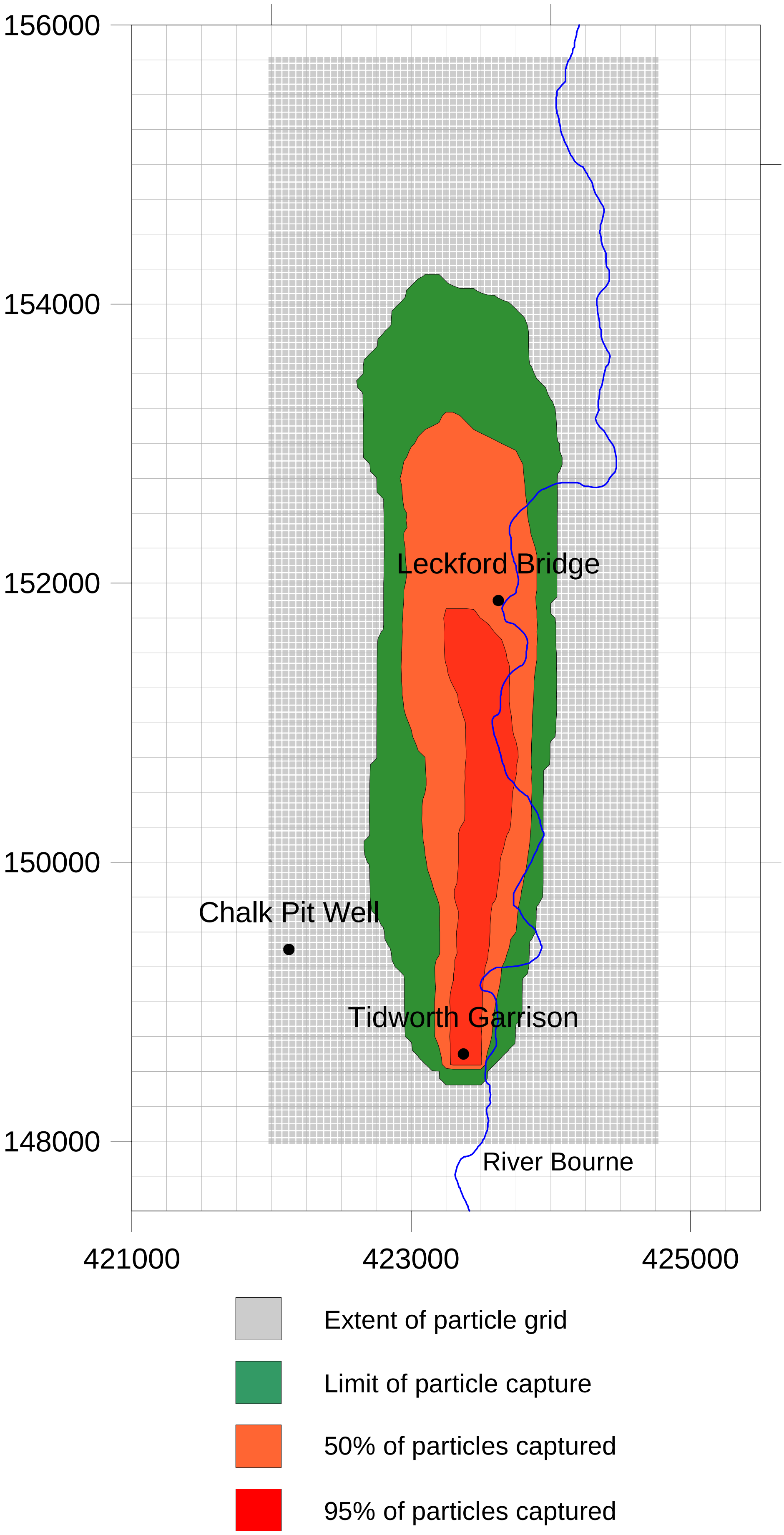
Issues with the technique include:

- 50 and 400-day time of travel zones have not been defined, although this should be possible.
- VKD is not fully taken into account – time variant depth averaged particle tracking is performed.

- The whole model cannot be analysed at once due to the large number of particles required. This may be overcome to a degree by increasing the particle spacing, or by small modifications to MODPATH to do the capture counting internally.
- A period of time is required after the final particle release for particles to be captured by the pumped well. A simple way to implement this in Chalk models is to cease releasing particles for a number of years (1-3) prior to the end of the flow simulation. In aquifers with higher residence times, e.g. Sherwood Sandstone, this may cause problems.

5

Figure 4.1 Time variant probability of capture zone for Tidworth Garrison



Conclusions and recommendations

5.1 Conclusions

The following conclusions are drawn from the tasks completed.

5.1.1 Time instant steady state (TISS) models and particle tracking

- TISS models completed under maximum and minimum groundwater conditions show theoretical extremes of capture zones.
- This approach is limited since the groundwater systems modelled have large seasonal variations and never reach either extreme steady state.
- It may be possible to create an average condition with which to conduct tracking, but this would not make full use of the time variant aspect of Regional models.

5.1.2 Effect of VKD on particle tracks

- The application of MODPATH to a MODFLOW-VKD model already takes VKD into account, to some extent, by using depth averaged velocities.
- Taking full account of the vertical variation in velocity using a VKD correction factor, as used in ZOOPT, changes the magnitude of the groundwater velocity vector while the direction of flow remains unchanged.
- With steady state VKD models of the Bourne catchment, taking account of differences in velocity at different elevations results in significant differences in pathlines, e.g. +100% for 50 and 400 day pathlines.
- The VKD velocity correction methodology developed can only be applied to steady state isotropic models without changes to the MODPATH source code.
- The VKD velocity correction methodology works, but the resultant time of travel zones and capture zones are unrepresentative because the model is steady state.

5.1.3 Time variant particle tracking

The investigation of time variant particle tracking has demonstrated that this technique is feasible and has significant advantages over steady state methods:

- A method has been developed to post process a multi release time, forward tracking model, so that a probabilistic capture zone plot for an abstraction can be produced.
- Full account is taken of the seasonal variations in recharge, heads and velocities within the aquifer.
- The resulting capture zone contains a probability distribution of “temporal likelihood” that a location falls within capture zones of an abstraction.
- The technique is equally applicable to aquifers other than the Chalk.

Unresolved issues with the technique include:

- 50 and 400-day time of travel zones are not defined, although this should be possible.
- VKD is not fully taken into account – particle tracking is performed using time variant depth averaged velocities.
- The whole model (spatially and temporally) cannot be analysed at once due to the large number of particles required. This may be overcome to a degree by increasing

the particle spacing, or by modifications to the MODPATH source code to do the capture counting internally.
- A period of time is required after the final particle release for particles to be captured by the pumped well. A simple way to implement this is to cease releasing particles for a number of years (1-3) prior to the end of the flow simulation. This may be an issue in other aquifer systems such as the Sherwood Sandstone with greater residence times.

5.2 Recommendations

The following recommendations are made:

- Time instant steady state models are not recommended as a way forward for source protection zones or other particle tracking applications.
- TISS models are slow to construct and remove the time variant nature of Regional models.
- Constructing TISS models at the extremes of groundwater fluctuation gives unrealistic particle tracks and protection zones that do not reflect the time variant nature of aquifer systems.
- This recommendation is particularly important in aquifers that exhibit a high degree of seasonal variation such as the Chalk.

- The ZOOPT VKD correction method does work and could be implemented with MODPATH for particle tracking with VKD. The following points are made regarding this option:
    - The effort involved in incorporating VKD into MODPATH, including testing, is estimated to be in the region of 40 to 80 person days or approximately £15-30k.
    - For some applications, the depth averaged velocity approximation used by MODPATH will be sufficient – given other uncertainties inherent in Regional Chalk models besides those associated with VKD.
    - Issues concerning time variant particle tracking would also have to be resolved, this is taken into account in the budget estimate.
    - To fully account for VKD, MODPATH would need access to information concerning VKD parameters (K_{base}, VKMID and VKMAX) and time variant groundwater heads. The elevation of particle release would also need to be specified.
    - Rather than concentrate solely on VKD more value may possibly be achieved by considering time variant particle tracking as a priority and taking account of the results of other studies into protection zone delineation such as Robinson and Barker, 2000.

- A time variant particle tracking methodology for application with Regional water resource models should be developed by the Agency:

    - The technique illustrated in Section 4 should be considered as one potential methodology for source protection zone and other particle tracking tasks with Regional models.

- Unresolved problems related to the technique have been described. It is anticipated that the majority of these can be overcome.
- The forward tracking approach illustrated in Section 4 can certainly be improved by modifications to the MODPATH code and could be developed to a fully functional methodology for time variant particle tracking. It is estimated that this would require 30-60 person days or approximately £10,000-20,000 if completed as a stand-alone project.
- There is also the possibility that time-variant backward tracking could be successfully implemented. Since this method has the potential to be simpler to use, any time variant particle tracking project should explore the feasibility of this method prior to further development of the forward tracking technique.

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List of abbreviations

GPZ	Groundwater Protection Zones
GWV	Groundwater vulnerability
SPZs	Source Protection Zones
TISS	Time Instant Steady State
USGS	United States Geological Survey

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