STOCHASTIC ANALYSIS OF CAPTURE ZONES

with varying parameters under heterogeneous conditions

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Abstract

Studies into well capture zones play an important role in resolving environmental and public health issues. Such issues include the determination of protection areas for drinking water wells and maximising the efficiency of hydraulic containment in contaminant extraction wells. The size, shape and location of a capture zone depend largely on the hydrogeologic properties of the aquifer and the characteristics of the extraction well. Some aquifer properties such as hydraulic conductivity are particularly prone to uncertainty due to heterogeneity. A stochastic approach can be used to characterise this uncertainty in a capture zone instead of the traditional deterministic approach.

Previous studies on the influence of aquifer and well properties on well capture zones were mostly carried out under the assumption of homogeneous hydraulic conductivity. In this work, the heterogeneity in aquifer hydraulic conductivity is modeled through a computer algorithm program (FGEN) that generates two-dimensional cross-correlated random fields. Capture zone probability distributions (capd) are used to investigate the changes in uncertainty of a fully confined two-dimensional capture zone in steady state due to changes in aquifer and well properties. Aquifer properties include hydraulic conductivity variance, soil hydraulic conductivity correlation lengths, anisotropic conditions and the hydraulic gradient. Well characteristics include the number of wells, the location of the wells and pumping (extraction) rates. These results are compared to the results derived from the traditional homogeneous assumption and normalised to reflect the influence of heterogeneity conditions.

Primary investigation into the capd showed that uncertainty in the capture zone increases with increasing variance in hydraulic conductivity and increasing anisotropic correlation length in the perpendicular direction. As the isotropic correlation length increases, uncertainty also increases, but decreases as the correlation length increases past a certain point. Normalised results also showed that uncertainty increases with increasing aquifer hydraulic gradient.

Different well pumping (extraction) rates were investigated with different hydraulic conductivity variances. The results indicate that with increasing variance, decreasing the pumping rates causes higher uncertainty. The influences of the location and number of wells on the capd were also investigated via dual extraction well numerical simulations.
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<th>Symbol</th>
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<tr>
<td>a</td>
<td>arbitrary constant</td>
</tr>
<tr>
<td>b</td>
<td>arbitrary constant</td>
</tr>
<tr>
<td>C, C_1, C_2</td>
<td>arbitrary coefficients</td>
</tr>
<tr>
<td>C_{10}</td>
<td>coefficient used to predict the behaviour of P10</td>
</tr>
<tr>
<td>C_{90}</td>
<td>coefficient used to predict the behaviour of P10</td>
</tr>
<tr>
<td>capd</td>
<td>capture zone probability distribution</td>
</tr>
<tr>
<td>C_L</td>
<td>correlation length</td>
</tr>
<tr>
<td>C_{LX}</td>
<td>correlation length in the x direction (perpendicular to the hydraulic gradient)</td>
</tr>
<tr>
<td>C_{LY}</td>
<td>correlation length in the y direction (parallel to the hydraulic gradient)</td>
</tr>
<tr>
<td>C_{LX}/C_{LY}</td>
<td>anisotropic ratio of the correlation length in the x direction divided by the correlation length in the y direction</td>
</tr>
<tr>
<td>( \nabla h )</td>
<td>hydraulic gradient</td>
</tr>
<tr>
<td>K</td>
<td>hydraulic conductivity</td>
</tr>
<tr>
<td>L</td>
<td>unit of length</td>
</tr>
<tr>
<td>L_i</td>
<td>isoline bordering the probability of ‘i’</td>
</tr>
<tr>
<td>m</td>
<td>meters</td>
</tr>
<tr>
<td>M</td>
<td>unit of mass</td>
</tr>
<tr>
<td>MC</td>
<td>Monte Carlo</td>
</tr>
<tr>
<td>n_e</td>
<td>effective porosity</td>
</tr>
<tr>
<td>N_{MC}</td>
<td>number of Monte Carlo realisations</td>
</tr>
<tr>
<td>P</td>
<td>probability</td>
</tr>
<tr>
<td>P_{10}</td>
<td>probability of capture greater than 0.1</td>
</tr>
<tr>
<td>P_{50}</td>
<td>probability of capture greater than 0.5</td>
</tr>
<tr>
<td>P_{90}</td>
<td>probability of capture greater than 0.9</td>
</tr>
<tr>
<td>P_{\text{capture}}</td>
<td>probability of capture</td>
</tr>
<tr>
<td>pdf</td>
<td>probability density function</td>
</tr>
<tr>
<td>Q</td>
<td>well pumping (extraction) rate</td>
</tr>
<tr>
<td>Q_b</td>
<td>well base pumping (extraction) rate</td>
</tr>
<tr>
<td>s</td>
<td>second</td>
</tr>
<tr>
<td>s_{\text{capd}}</td>
<td>80 percent areal spread of the capture zone probability distribution</td>
</tr>
<tr>
<td>T</td>
<td>unit of time</td>
</tr>
<tr>
<td>t</td>
<td>time</td>
</tr>
<tr>
<td>x</td>
<td>spatial Cartesian coordinate x</td>
</tr>
<tr>
<td>y</td>
<td>spatial Cartesian coordinate y</td>
</tr>
<tr>
<td>z</td>
<td>spatial Cartesian coordinate y</td>
</tr>
<tr>
<td>( \Delta x )</td>
<td>grid discretisation (size)</td>
</tr>
<tr>
<td>( \mu )</td>
<td>statistical mean</td>
</tr>
<tr>
<td>( \mu_K )</td>
<td>statistical mean of hydraulic conductivity</td>
</tr>
<tr>
<td>( \sigma^2 )</td>
<td>standard deviation</td>
</tr>
<tr>
<td>( \sigma^2 )</td>
<td>variance</td>
</tr>
<tr>
<td>( \sigma^2_K )</td>
<td>variance of hydraulic conductivity</td>
</tr>
<tr>
<td>( \rightarrow )</td>
<td>approaches</td>
</tr>
<tr>
<td>( \infty )</td>
<td>infinity</td>
</tr>
<tr>
<td>( \approx )</td>
<td>approximately equals</td>
</tr>
<tr>
<td>( \Sigma )</td>
<td>the sum of</td>
</tr>
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Chapter 1

Introduction
1 Introduction

The accurate description of well capture zones plays an important role in well head protection and designing remediation systems for contaminated aquifers. Protection is a relative concept in the sense that it implies degrees of protection (Zhang 2002). A higher level of protection implies a lower acceptable risk of damage to the protected quantity. In a risk assessment analysis, potential sources of contamination are identified and evaluated in terms of probability of occurrence and amount of resulting damage.

Well capture zones are generally estimated using analytical or numerical models based on a homogeneous aquifer assumption. However, aquifers exhibit large degrees of heterogeneity due to the complex geological processes through which natural formations evolve. This hampers a complete determination of the aquifer properties and introduces uncertainty in capture zone delineation.

Solutions that describe a capture zone using a homogeneous assumption are deterministic and obscure the uncertainty associated with heterogeneity. Stochastic simulations can be used to characterise heterogeneity and provide a formal framework for the analysis of uncertainty through probability distributions within the resulting capture zone. This gives a more “honest” representation of the capture zone and relates to the concept that groundwater protection is assessed through the level of risk.

This thesis uses a stochastic modelling approach to represent aquifer heterogeneity based on the statistical variance and correlation structure of the soil. Under these conditions, different aquifer and well properties are varied to observe their effects on the resulting level of uncertainty in the capture zone. Changes in the behaviour of uncertainty will be qualitatively and quantitatively described in terms of probability. The deviation of the capture zones derived under heterogeneous conditions will be measured against the expected equivalent homogeneous capture zones.
1.1 Problem Definition

The influence of different aquifer and well properties on capture zones has been studied in the past under the assumption of homogeneous, isotropic aquifers. These studies generally provide an analytical description of the effects of changing aquifer and well parameters on the capture zone. In a confined aquifer these parameters include the hydraulic conductivity, the hydraulic gradient and the well pumping rate. The direct application of these analytical methods to real cases is, however, limited by its underlying assumptions – mainly those of a homogeneous and isotropic domain.

Geostatistics can be used to simulate heterogeneity as a random space function through stochastic simulations. Past stochastic studies have focused solely on the effects of the variance and correlation structure of the heterogeneity on the extent of uncertainty about the location of a capture zone. There are no stochastic studies carried out to investigate the effects on uncertainty in the capture zone due to changing fundamental well and aquifer properties that affect the capture zone in homogeneous formulations.

This thesis provides a link between the past studies carried out under a homogeneous assumption and the stochastic simulations carried out using heterogeneous aquifers. The influence of different aquifer and well properties on capture zones will be studied under heterogeneous conditions. The effects of these parameters on the extent of uncertainty about the location of the capture zone will be assessed. Comparisons will be made to the equivalent homogeneous capture zones and the level of deviation will be quantified.

1.2 Thesis objectives

The general objectives of this thesis are as follows:

- To give a qualitative and quantitative description of the extent of uncertainty in the boundaries of large scale, two dimensional capture zones due to heterogeneity in hydraulic conductivity through stochastic simulations;
- To develop a general behavioural relationship between the size, shape, location and uncertainty of a capture zone due to increasing variance in heterogeneity and correlation structure of an aquifer;
• To give a qualitative and quantitative description of the extent of uncertainty when other aquifer properties are changed. These properties include anisotropic conditions and hydraulic gradient;
• To develop a general behavioural relationship between the size, shape, location and uncertainty of a capture zone due to changing anisotropic conditions and hydraulic gradient;
• To give a qualitative and quantitative description of the extent of uncertainty when other well properties are changed. These properties include the pumping rate, the number of wells and the location of wells;
• To develop a general behavioural relationship between the size, shape, location and uncertainty of a capture zone due to changing well properties and locations;
• To relate the results from the simulations and methodology in this thesis to its applications in the “real world”.

1.3 Thesis outline

Chapter 2 contains the background and literature review on groundwater flow, capture zone analysis and numerical modelling. It is aimed to review and summarise concepts that have direct relevance to this study. It also presents some limitations in past studies and concepts used in this thesis.

Chapter 3 presents a detailed methodology that was followed in this thesis. It describes the calibration of the numerical model and details of the stochastic methodology adopted. The chapter concludes with the results of a convergence test.

In chapter 4, the results and discussion give an insight into how aquifer and well properties influence the behaviour of uncertainty in a capture zone. Of particular interest is how the behaviour of the capture zone deviates from the homogeneous assumption.

This thesis is concluded in chapter 5 with a summary of the results, recommendations for practical application and suggestions for future work.
Chapter 2

Background and Literature review
2 Background and Literature review

Groundwater is an important source of water supply world wide and is used for many applications such as direct human consumption, industrial processes and agriculture irrigation. The main method of drawing groundwater for use is via extraction wells. When a pumping well abstracts water from its surrounding rock, it causes a local drawdown of the hydraulic head or the water table (van Leeuwen 2000). The area from which the well abstracts water from is called the capture zone. If a polluting event takes place in this area, the pollution will reach the well within a specified time span. The accurate determination of the well capture zone is therefore of great importance.

Groundwater contamination can be naturally occurring, but it is typically a result of land uses associated with modern society. Nearly anything that can be spilled or spread on the ground has the potential to leach or seep through the ground and into groundwater. The physical setting of an area usually determines how easily groundwater becomes contaminated if inadequate waste management or improper land uses occur.

2.1 Principles of groundwater flow

The flow of groundwater is controlled by the laws of physics and thermodynamics. Groundwater possesses energy in mechanical, thermal and chemical form. Since the amounts of energy vary spatially, groundwater is forced to move from one region to another in nature’s attempt to eliminate these energy differentials (Fetter 2001). In this thesis, it is assumed that the chemical energy is constant (water with constant temperature), thus allowing a separate examination of the effects of changing the mechanical energy in a system. Thermal energy must be considered, however, in such applications as geothermal flow systems and burial of radioactive heat sources. The major influencing factors that govern groundwater flow, with direct relevance to this thesis, are the aquifer/soil properties and the hydraulic head. The direction of groundwater flow is a function of the potential field, the degree of anisotropy of the hydraulic conductivity and the gradient of the hydraulic head (Fetter 2001).
2.1.1 Hydraulic Head

The hydraulic head is the mechanical energy that governs the movement of groundwater through the medium. Hydraulic head includes kinetic energy, gravitational potential energy and energy of fluid pressures and is shown in Equation 2-1:

\[
\frac{v^2}{2g} + z + \frac{P}{\rho g} = \text{cons tan } t
\]

**Equation 2-1**

Where \( v \) is the velocity of the fluid [L/T], \( z \) is the elevation head [L], \( P \) is the pressure [M/L/T\(^2\)], \( \rho \) is the density of the fluid [M/L\(^3\)], and \( g \) is the acceleration of gravity [L/T\(^2\)].

Since the flow of natural groundwater in the porous media has a very low velocity, the kinetic energy term \( (v^2/2g) \) becomes negligible relative to the other terms. The position of the fluid mass relative to a datum is the fluid’s gravitational potential energy, and is reflected in the term \( z \). Pressure acting from surrounding fluid can also contribute to potential energy, which is reflected in the term \( P / \rho g \).

For a fluid at rest, the pressure at a point is equal to the weight of the water above the point per unit cross sectional area. Equation 2-2 shows that the height of the water column, \( h_p \), provides a pressure head:

\[
P = \rho gh_p
\]

**Equation 2-2**

where \( h_p \) is the height of the water column above the point [L].

The hydraulic head is the sum of the elevation head and the pressure head. This is shown in Equation 2-3:

\[
h = z + h_p
\]

**Equation 2-3**

where \( h \) is the total hydraulic head [L].
The hydraulic head decreases in the direction of the flow of groundwater (Bear 1979). As the groundwater flows through a porous medium, some of the head is lost in the generation of heat as the fluid overcomes frictional resistance. Groundwater will flow from areas of high head to low head.

### 2.2 Aquifer and soil characteristics

The major properties of an aquifer with direct relevance to this study are defined in the following section. These aquifer properties influence the location and size of the capture zone in steady state, as well as uncertainty.

#### 2.2.1 Hydraulic Conductivity

Hydraulic conductivity ($K$) is an important hydrogeologic property as it describes the ease in which a fluid can flow through the porous media. It affects the flow paths and local groundwater velocities. The intrinsic permeability, defined as:

$$ K_i = C d^2 $$

**Equation 2-4**

where $K_i$ is the intrinsic permeability [L$^2$], $C$ is the dimensionless constant and $D$ is the mean diameter [L]. This relates to the size of the voids through which the fluid moves. The constant $C$ in Equation 2-4 describes the overall effect of the shape of the pore spaces (Fetter 2001). Hydraulic conductivity is related to the intrinsic permeability via Equation 2-5.

$$ K = K_i \left( \frac{\rho g}{\mu} \right) $$

**Equation 2-5**

where $K$ is the hydraulic conductivity [LT$^{-1}$], $K_i$ is the intrinsic permeability [L$^2$], $\rho$ is the density of the fluid [ML$^{-3}$], $g$ is the acceleration of gravity [LT$^{-2}$] and $\mu$ is the dynamic viscosity of the fluid [ML$^{-1}$T$^{-1}$].

It is a function of the properties of both the porous medium and the fluid flowing through it, such as the density and dynamic viscosity of the fluid. The dynamic viscosity of a fluid is the resistance of the fluid to the shearing necessary for fluid
flow (Fetter 2001). Table 2-1 shows the variation in hydraulic conductivity of different soil types.

<table>
<thead>
<tr>
<th>Material</th>
<th>Intrinsic permeability (darcys)</th>
<th>Hydraulic conductivity (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clay</td>
<td>(10^{-6} - 10^{-3})</td>
<td>(10^{11} - 10^{8})</td>
</tr>
<tr>
<td>Silt, sandy silts, clayey sands, till</td>
<td>(10^{-3} - 10^{-1})</td>
<td>(10^{8} - 10^{6})</td>
</tr>
<tr>
<td>Silty sands, fine sands</td>
<td>(10^{-2} - 1)</td>
<td>(10^{7} - 10^{5})</td>
</tr>
<tr>
<td>Well sorted sands, glacial outwash</td>
<td>(1 - 10^2)</td>
<td>(10^{5} - 10^{3})</td>
</tr>
<tr>
<td>Well-sorted gravel</td>
<td>(10 - 10^3)</td>
<td>(10^{4} - 10^{1})</td>
</tr>
</tbody>
</table>

Table 2-1 Ranges of intrinsic permeabilities and hydraulic conductivities for unconsolidated sediments (modified from Fetter 2001, p85)

With all other properties being equal, groundwater flow is greatest in sediments with a high hydraulic conductivity, such as sand and gravel, in comparison to clay.

### 2.2.2 Saturated Thickness

The saturated thickness, \(b\), of the aquifer is equal to the thickness of the aquifer in the case of a fully saturated, confined aquifer, or equal to the distance between the aquifer base and the water table in the case of an unconfined aquifer.

### 2.2.3 Transmissivity

Transmissivity measures the amount of water transmitted through a unit width of the saturated thickness of an aquifer under a unit hydraulic gradient. It is defined by the product of the hydraulic conductivity and the saturated thickness of the aquifer (Fetter 2001) as seen in Equation 2-6 below. Flow in the aquifer is assumed to be horizontal.

\[ T = bK \]

**Equation 2-6**

\(T\) is the transmissivity \([L^2T^{-1}]\), \(b\) is the saturated thickness of the aquifer \([L]\) and \(K\) is the hydraulic conductivity \([LT^{-1}]\).
2.2.4 Effective porosity

The porosity of earth materials is the percentage of the rock or soil that is void of material (Fetter 2001). It is defined by the following equation:

\[ n = \frac{100V_v}{V} \]

Equation 2-7

where \( n \) is the porosity (percentage), \( V_v \) is the volume of void space in a unit volume of earth material \([L^3]\) and \( V \) is the unit volume of earth material, including both voids and solids \([L^3]\).

Effective porosity, \( n_e \), is the porosity available to fluid flow. Past studies into effective porosity of fine grained sediments came to the conclusion that \( n_e \) is a function of the size of molecules that are being transported relative to the passageways that connect the pores (Fetter 2001). The total porosity can be computed from the relationship

\[ n = 100\left[1 - \left(\frac{\rho_b}{\rho_d}\right)\right] \]

Equation 2-8

where \( n \) is the total porosity as a percentage, \( \rho_b \) is the bulk density of the aquifer material \([ML^{-3}]\) and \( \rho_d \) is the particle density of the aquifer material \([ML^{-3}]\).

Porosity can be estimated using knowledge of rock type or by performing laboratory tests on core samples. The general range of porosity that can be expected for typical sediments is listed in Table 2-2 (Fetter 2001).

**Table 2-2 Porosity ranges for sediments – from Fetter 2001, pp75**

<table>
<thead>
<tr>
<th>Sediment type</th>
<th>Porosity Ranges</th>
</tr>
</thead>
<tbody>
<tr>
<td>Well-sorted sand or gravel</td>
<td>25-50%</td>
</tr>
<tr>
<td>Sand and gravel, mixed</td>
<td>20-35%</td>
</tr>
<tr>
<td>Glacial till</td>
<td>10-20%</td>
</tr>
<tr>
<td>Silt</td>
<td>35-50%</td>
</tr>
</tbody>
</table>
2.3 Groundwater Flow Equation

There are several important governing equations for groundwater flow. Darcy’s Law can be used to describe flow through a porous medium in its one-dimensional form. In three dimensions, groundwater flow equations are based on the conservation of energy and mass laws and Darcy’s Law. These equations describe groundwater flow under natural forces. A confined aquifer is used as this has direct relevance to the work presented in this thesis.

2.3.1 Darcy’s Law

Darcy’s Law describes the flow of water in a prism of porous material, and is defined in its one-dimensional form in Equation 2-9. Discharge is proportional to the cross-sectional area of the prism and the hydraulic conductivity of the material (Fetter 2001).

\[
Q = -\frac{KA(h_2-h_1)}{L}
\]

Equation 2-9

Q is the volumetric flow \([L^3 T^{-1}]\), K is the hydraulic conductivity \([LT^{-1}]\), A is the cross-sectional area perpendicular to the flow \([L^2]\), \((h_2-h_1)\) is the head difference parallel to the flow \([L]\) and L is the length of the flow path \([L]\).

The greater the change in hydraulic head between two points, the larger the volumetric flow. The hydraulic gradient is defined as the head difference at two points divided by the length of the flow path (Fetter 2001). Discharge is inversely proportional to the length of flow, L. The flow is in the direction of the decreasing hydraulic gradient, or from high head to low head (Fetter 2001). This is represented by the negative sign in Equation 2-9.

Darcy’s law applies for very slowly moving groundwater and is only valid for conditions where the resistive forces of viscosity dominate (Fetter 2001). In most natural groundwater systems, the velocity of the groundwater flow is low enough that
Darcy’s law is valid. Areas of rocks with large openings, such as solution openings, and steep hydraulic gradients, such as adjacent to pumping wells, are situations where Darcy’s law is not valid (Fetter 2001).

The Darcy flux or specific discharge is the velocity of the groundwater if it was flowing through an open pipe, instead of through pore voids (Fetter 2001). It is defined in Equation 2-10:

\[ q = \frac{Q}{A} \]

**Equation 2-10**

where \( q \) is the specific discharge \([LT^{-1}]\).

Groundwater flows through a cross-sectional area in a porous medium that is smaller than the dimensions of the aquifer. This is due to the fact that groundwater can only move through interconnected pore spaces. The effective porosity is the portion of the pore space through which saturated flow occurs. This is used to calculate the average rate that groundwater moves, known as the seepage velocity or average linear velocity shown in Equation 2-11:

\[ V_x = \frac{Q}{n_e A} \]

**Equation 2-11**

where \( V_x \) is the average linear velocity \([LT^{-1}]\) and \( n_e \) is the effective porosity.

### 2.3.2 Three-dimensional Groundwater Flow

The laws of conservation of mass and energy are combined with Darcy’s Law to derive the differential equations describing groundwater flow in the porous media. The equations describe flow using independent spatial coordinates, \( x, y, z \) and time, \( t \) (Fetter 2001).
The three-dimensional groundwater flow equation for a heterogeneous, anisotropic confined aquifer is defined in Equation 2-12 below. This equation applies to transient situations, where the flow varies with time.

\[
\frac{\partial}{\partial x} \left( K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial h}{\partial z} \right) = S_x \frac{\partial h}{\partial t}
\]

Equation 2-12

In steady state flow, there is no change with head in time as the water table slope or position remains constant (Fetter 2001). The equation can be simplified and is shown in Equation 2-13.

\[
\frac{\partial}{\partial x} \left( K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial h}{\partial z} \right) = 0
\]

Equation 2-13

### 2.3.3 Groundwater Flow to Wells

An extraction or injection well is a point sink or source affecting the overall natural flow pattern of an aquifer (Bear 1979). In a homogeneous and isotropic aquifer, radial flow occurs due to a well (Fetter 2001). If a well is used to extract water from an aquifer, then there will be a decrease of head or drawdown in the aquifer around the well. A build-up or increase in head will result due to an injection well.

Flow is initially unsteady as the head changes with time if water is injected into or pumped from an aquifer. This will result in a growing cone of depression or build-up forming in the aquifer around the well (Fetter 2001). When a source or sink is intercepted by the growing cone of depression or build-up respectively, the cone of depression or build-up remains constant with time, and steady flow occurs (Fetter 2001). For an injection well, sinks may include water bodies such as nearby rivers or leakage to other aquifers.

The following assumptions are made in the following sections in the derivation of the equations for groundwater flow due to wells (Fetter 2001):

- The geologic formations and groundwater flow are horizontal;
• The head of the aquifer was at steady state before pumping, and only changes due to the effects of pumping;
• Darcy’s Law is valid;
• The well is screened over the entire thickness of the aquifer;
• The aquifer is confined.

In a confined aquifer, water is obtained from the elastic storage of the aquifer which is measured by the storativity. Equation 2-14 describes the radial flow due to a well in a confined aquifer:

\[
\frac{\partial^2 h}{ \partial r^2 } + \frac{1}{r} \frac{\partial h}{\partial r} = \frac{S}{T} \frac{\partial h}{\partial t}
\]

Equation 2-14

where \( h \) is the hydraulic head [L], \( S \) is the storativity, \( T \) is transmissivity [L^2T^{-1}], \( t \) is time [T] and \( r \) is the radial distance from the well [L]. Equation 2-14 is given in radial coordinates (Fetter 2001).

The Theis equation is a solution to Equation 2-14 (Fetter 2001). It is assumed that the potentiometric surface is initially horizontal and the aquifer extends in the horizontal direction infinitely. Equation 2-15 and Equation 2-16 shows the Theis equation:

\[
h_0 - h = \frac{Q}{4\pi T} W(u)
\]

Equation 2-15

where \( W(u) \) is the well function and has tabulated values for various \( u \) values and:

\[
u = \frac{r^2 S}{4 T t}
\]

Equation 2-16

where \((h_0-h)\) is the drawdown at a certain point [L], \( Q \) is the pumping rate [L^3T^{-1}], \( T \) is the transmissivity [L^2T^{-1}], \( t \) is the elapsed time of pumping [T], \( S \) is the aquifer storativity and \( r \) is the distance from the well [L].
Equation 2-14 to Equation 2-16 are based on several assumptions including total aquifer confinement (no recharge), constant rate of well pumping and the aquifer is compressible and water is released immediately as the head decreases. The Theis or non-equilibrium curve is a graphical solution which plots \( W(u) \) as a function of \( 1/u \) on a logarithmic scale. Field data for a drawdown versus time will lie on this curve if the aquifer is homogeneous and isotropic.

An aquifer or pump test can be used to determine aquifer parameters in the vicinity of the pumping or injection well (Bear 1979). These parameters may include the radial anisotropy, transmissivity and storativity. The presence of recharge or barrier boundaries may also be sought. The parameters are used to predict the buildup by an injection well (Fetter 2001). As a well is pumped at a constant rate, the rate of drawdown of the water level in nearby observation wells is monitored. The time-drawdown data is used to obtain the hydraulic parameters of the aquifer (Fetter 2001).

### 2.4 Capture zone analysis

A capture zone can be defined as the up-gradient and down-gradient areas that will be drawn into a pumping (extraction) well. The capture zone will correspond to the cone of depression if the water table is perfectly flat (Fetter 2001). However, in most cases the water table is sloping, so the capture zone will not correspond to the cone of depression. The capture zone will be an elongated area that extends slightly down-gradient of the pumping well and extends in an up-gradient direction. The capture zone area is controlled by the time that it takes for water to flow from an up-gradient area to the pumping well. In a steady state case, where sufficient pumping time elapses, the capture zone will eventually extend up-gradient to the closest water divide.

To protect the quality of water draining towards municipal supply wells, well head protection zones are being defined in many communities (Guadagnini and Franzetti 1999). Land uses that may result in groundwater contamination are being regulated in the well protection zones. The capture zone of an extraction well is equivalent to a well head protection zone of a water supply well.
The cross section of an unconfined aquifer with a sloping water table is shown in Figure 2-1.

Figure 2-1: Plan and cross-section view of a capture zone. This example was taken from Cohen et. al. (1994) and is a capture zone created from hydraulic containment using a pumping well.

The cone of depression of the pumping well will reverse the hydraulic gradient for a short distance down-gradient of the well. Thus, the capture zone extends for a short distance down-gradient of the well. A ground water divide surrounds the entire capture zone where outside the divide, the flow will pass the well, and inside the divide, the flow will be drawn into the well (Cohen et. al 1994).

2.4.1 Methods of determining the capture zone

The traditional ways in determining the capture zone are through analytical or numerical methods. They will be briefly discussed in the following sections.

2.4.1.1 Analytical methods

Simple analytical description of the location of capture zones can only be found for cases where there is either a zero background gradient or zero recharge. In the case of zero background gradient and zero recharge, the analytical description of the capture zone is equivalent to that described in Section 2.3.3. In most cases, analytical solutions assume isotropic and homogeneous hydraulic conductivity and effective porosity, as well as confined flow conditions.
The analytical description for the edge of the capture zone for a confined aquifer when steady state conditions have been reached is given in Equation 2-17 (Grubb 1993):

\[
x = \frac{-y}{\tan(2\pi K b i y / Q)}
\]

Equation 2-17

where \(x\) and \(y\) represent the 2 dimensional directions in a traditional Cartesian coordinate system, \(Q\) is the pumping rate (\(L^3/T\)), \(K\) is the hydraulic conductivity (\(L/T\)), \(b\) is the initial saturated thickness of the aquifer (\(L\)), \(i\) is the hydraulic gradient of the flow field in the absence of the pumping well (dimensionless) and \(\tan(y)\) is in radians.

From Equation 2-17, the distance from the pumping well downstream to the stagnation point that marks the end of the capture zone is given by Equation 2-18:

\[
x_0 = -\frac{Q}{(2\pi K b i)}
\]

Equation 2-18

where \(x_0\) is the distance from the pumping well to the down-gradient edge of the capture zone (\(L\)). The maximum width of the capture zone as \(x\) approaches infinity is given by Equation 2-19:

\[
y_{\text{max}} = \pm\frac{Q}{(2K b i)}
\]

Equation 2-19

where \(y_{\text{max}}\) is the half-width of the capture zone as \(x\) approaches infinity.

Grubb (1993) gave a solution to the capture zone in an unconfined aquifer. The shape of the capture zone is given by Equation 2-20:

\[
x = \frac{-y}{\tan[\pi K (h_i^2 - h_2^2) y / Q L]}
\]

Equation 2-20
where other parameters are the same as before and $h_1$ is the up-gradient head, $h_2$ is the down-gradient head and $L$ is the distance between the two monitoring wells. From Equation 2-20, the maximum width of the capture zone as $x$ approaches infinity and position of the stagnation point can be calculated. Since this thesis deals with confined aquifer simulations, the details will not be discussed here.

For transient (non-steady state) cases, Bear and Jacobs (1965) derived analytical solutions for the isochrones of a steady pumping well in an isotropic, homogeneous, confined aquifer with uniform background flow. For the purely advective transport of an ideal tracer the isochrones are defined in Equation 2-21:

\[
\hat{t} = x + \ln\frac{\sin \theta}{\sin(y + \theta)} \quad \theta = \arctan(y/x)
\]

where $x$ is the distance from the well in the direction of the background flow and $y$ is the distance from the well, at right angles to this direction, of the location of a pulse injection; $(\hat{x}, \hat{y}, \hat{t})$ (see Figure 2-2) are the corresponding dimensionless coordinates, which result from the following transformations in Equation 2-22:

\[
\hat{x} = \frac{x}{Q/(2\pi q_0)} \quad \hat{y} = \frac{y}{Q/(2\pi q_0)}
\]

where $Q$ ($L^2/T$) is the extraction rate per unit thickness of aquifer, $n$ is porosity, $q_0=K_j_0$ ($L/T$) is the Darcy’s natural flow velocity and $j_0$ is the background uniform gradient. From Equation 2-21 and Equation 2-22, the dimensionless quantities are obtained as ratios to the stagnation point distance from the well.
It can be shown that the location of the groundwater divide is given by Equation 2-23 (Bear and Jacobs 1965):

$$\bar{x} = -\frac{\bar{y}}{\tan \bar{y}}$$

Equation 2-23

which is derived from Equation 2-21 and Equation 2-22 in the limit $\bar{t} \to \infty$; the asymptotic width of the wellhead influence region is

$$\bar{y} = \pm \pi \quad \text{when} \quad \bar{x} \to \infty.$$ 

The isochrones in Figure 2-2 indicate travel time $\bar{t}$ to the well and the groundwater divide is the particular isochrone $\bar{t} \to \infty$. When the time approaches infinity, the capture zone is equivalent to Equation 2-17 for steady state conditions. Learner (1992) further extended this work and developed an analytical solution which takes into account areally homogeneous recharge so as to delineate the shapes of catchments and isochrones, for a well bounded homogeneous domain, in the case of purely advective solute movement.
The direct application of these analytical methods to real cases is limited by its underlying assumptions, mainly those of a homogeneous and isotropic domain and purely advective transport, assumptions which are seldom applicable to natural aquifers. Bhatt (1993) carried out a sensitivity analysis showing that errors in the measurement of field parameters (porosity, saturated thickness, hydraulic conductivity and natural gradient) have a strong impact on the results.

2.4.1.2 Numerical methods

Numerical models start with the basic groundwater flow equation (Equation 2-12). This is solved for the head distribution in the aquifer. Determining the capture zone through numerical methods is usually based on the analysis of flow paths, whereby the ensemble of flow paths ending in the well is defined as the catchment. Analysis of travel times along the flow paths allows for the determination of time-related capture zones (van Leeuwen 2000). This method is referred to as “particle tracking”, as a flow path describes the path along which a virtual particle travels when it is released at the starting point of the flow path. The equation of a flow path in a three-dimensional flow field is given by

\[
\frac{dx(t)}{dt} = v_x, \quad \frac{dy(t)}{dt} = v_y, \quad \frac{dz(t)}{dt} = v_z,
\]

where \(v_x\), \(v_y\) and \(v_z\) are the average linear velocities in the \(x\), \(y\) and \(z\) directions at a point. These velocities can have several components, attributed to, for example, recharge, regional flow, or pumping wells.

There are two ways in which particle tracking can be used to determine capture zones—forward and backward tracking (van Leeuwen 2000). In forward particle tracking, particles are released at the beginning of flow paths, for example at the top surface of all grid cells in the area of interest. In backward particle tracking, particles are released at the end points of flow paths, that is, in the vicinity of the well. An advantage of the forward tracking method is that particle end points and travel times are calculated for all grid cells, providing a precise definition of isochrone locations.
With the backward tracking method, the isochrone distribution is only defined at the locations visited by the flow paths, resulting in a less precise definition of the isochrone locations. The advantage of backward tracking is that only a few particles need to be released in order to get a good first impression of the location of the isochrones, reducing calculation time.

2.5 Heterogeneity in formations

2.5.1 Assumptions of homogeneity and isotropy

Of the methods review in the previous section, all of them made the assumption that the field is homogeneous and isotropic. A homogeneous unit is one that has the same property at all locations (Fetter 2001). In an aquifer, this would indicate that the grain size distribution, porosity, degree of cementation and thickness are variable only within small limits. The values of the transmissivity and storativity of the unit would be about the same wherever present. In non-homogeneous formations, or heterogeneous formations, hydraulic properties change spatially.

In a porous medium made of spheres of the same diameter packed uniformly, the geometry of the voids is the same in all directions. Thus, the intrinsic permeability of the unit is the same in all directions, and the unit is said to be isotropic (Fetter 2001). Conversely if the geometry of the voids is not uniform, there may be a direction in which the intrinsic permeability is greater. The medium is thus anisotropic. A porous medium composed of book shaped grains arranged in a subparallel manner would have a greater permeability parallel to the grains than crossing the grain orientation. This is shown in Figure 2-3.

![Figure 2-3: Grain shape and orientation affects permeability in a given direction. The left side shows isotropic sediments while the right side shows anisotropic sediments.](image-url)
2.5.2 Heterogeneity and uncertainty

The size, shape and location of a capture zone are largely determined by the hydrogeological properties of the local aquifer and the characteristics of the pumping well (van Leeuwen 2000). The characteristics of the pumping well are usually well known and controllable but the hydrogeological properties are often difficult to assess. This creates uncertainty in the capture zone.

The main aquifer properties influencing steady state groundwater flow are hydraulic conductivity, saturated thickness and effective porosity. Other parameters include recharge and location of aquifer boundaries. Recharge of the aquifer by infiltrating rainwater or by other sources such as streams and lakes can decrease the size of the capture zone because it provides a pumping well with water not only from horizontal flow, but also from vertical flow (van Leeuwen 2000). The amount and spatial distribution of recharge becomes difficult to assess, especially under complex permeability structures, and adds considerable uncertainty to the analysis of the capture zone. Since this work deals with a fully confined aquifer with no recharge, the uncertainty is not influenced by recharge but nevertheless its importance should not be neglected.

All the aforementioned aquifer properties exhibit a certain degree of heterogeneity and unpredictable spatial variability. As a result they are often not completely obtainable and practically impossible to measure at all locations. In most cases, this creates the highest uncertainty in groundwater flow modeling (van Leeuwen 2000). Of all the aquifer properties mentioned above, hydraulic conductivity is often the most important as its variability in space is considerably higher than that of other properties. Hydraulic conductivity can vary by orders of magnitude over a few meters (van Leeuwen 2000). Other parameters such as effective porosity are typically more homogeneous in any one particular aquifer and its maximum range of variation (15%-35%) is significantly less than that of hydraulic conductivity.
2.5.3 Scales of heterogeneity

Heterogeneity properties of hydraulic conductivity can be defined for different scales. The scale at which aquifer properties are described in groundwater flow models should depend on the scale of the problem considered (van Leeuwen 2000).

A convenient classification of scales introduced by Dagan (1986) consisted of the following length scales. The core scale, in order of $10^{-1}$-100 meters, is the minimum scale considered. This is the scale at which measurements of hydraulic conductivity and effective porosity are taken, using undistributed soil samples. The local or formation scale, in order of $10^2$-$10^3$ meters, is related to the thickness of the aquifer and to a similar dimension in the plane. Groundwater flow in this scale is generally three-dimensional and heterogeneity is associated with, for example, layering in sedimentary formations. The regional scale, in order of $10^3$-$10^5$ meters, is related to the entire aquifer or formation. The horizontal dimension in this scale is much larger than the vertical. This scale is relevant, for example, to the exploitation of aquifers and to well catchments. At this scale aquifer properties can be averaged over the aquifer thickness, representing them as two dimensional (van Leeuwen 2000). Figure 2-4 and Figure 2-5 shows heterogeneity on different scales.

Figure 2-4: Small scale heterogeneity (van Leeuwen 2000).
2.5.4 Representing heterogeneity and anisotropy

The regional scale is most relevant to the investigations carried out in this thesis. In the regional scale, capture zones are assumed to be at a scale at which the vertical dimension is small compared to the horizontal dimension. The relevant scale dependent statistical parameters of hydraulic conductivity variation are the variance and the correlation length. These values are based on the natural-log normal distribution and will be discussed in the next section.

For a number of aquifers in the United States and Europe these statistical parameters have been investigated and results have been published (e.g. Hoeksema and Kitanidis 1985). Table 2-3 summarises some data from different sites, relevant for different scales.
Table 2-3: Values of variance and correlation lengths for different aquifer types and different scales (Gelhar 1993).

<table>
<thead>
<tr>
<th>Medium</th>
<th>( \sigma^2 )</th>
<th>Correlation scale (m)</th>
<th>Overall scale (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Horizontal</td>
<td>Vertical</td>
</tr>
<tr>
<td>1. Local scale: two dimensions</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sandstone aquifer</td>
<td>1.5–2.2</td>
<td>0.3–1.0</td>
<td>14</td>
</tr>
<tr>
<td>Fluvial sand</td>
<td>0.9</td>
<td>&gt; 3</td>
<td>0.1</td>
</tr>
<tr>
<td>Aeolian sandstone outcrop</td>
<td>0.4</td>
<td>8</td>
<td>3</td>
</tr>
<tr>
<td>Glacial outwash sand</td>
<td>0.5</td>
<td>5</td>
<td>0.36</td>
</tr>
<tr>
<td>Sand and gravel aquifer</td>
<td>4.9</td>
<td>20</td>
<td>0.5</td>
</tr>
<tr>
<td>Fluvial sand and gravel aquifer</td>
<td>2.1</td>
<td>13</td>
<td>1.5</td>
</tr>
<tr>
<td>Glacial outwash sand and gravel outcrop</td>
<td>0.8</td>
<td>5</td>
<td>0.4</td>
</tr>
<tr>
<td>Glacial-lacustrine sand aquifer</td>
<td>0.6</td>
<td>3</td>
<td>0.12</td>
</tr>
<tr>
<td>2. Local scale: one dimension</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fluvial soil</td>
<td>1.0</td>
<td>7</td>
<td>6</td>
</tr>
<tr>
<td>Prairie soil</td>
<td>0.6</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td>Weathered shale subsoil</td>
<td>0.8</td>
<td>&lt; 2</td>
<td></td>
</tr>
<tr>
<td>Honarzed Mediterranean soil</td>
<td>0.4–1.1</td>
<td>14–39</td>
<td></td>
</tr>
<tr>
<td>Gravelly loamy sand soil</td>
<td>0.7</td>
<td>500</td>
<td></td>
</tr>
<tr>
<td>Alluvial silty-clay loam soil</td>
<td>0.6</td>
<td>0.1</td>
<td></td>
</tr>
<tr>
<td>Alluvial soil (Yolo)</td>
<td>0.9</td>
<td>15</td>
<td></td>
</tr>
<tr>
<td>3. Regional scale: one dimension</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Alluvial-basin aquifer</td>
<td>1.22</td>
<td>4,000</td>
<td></td>
</tr>
<tr>
<td>Alluvial-basin aquifer</td>
<td>1.0</td>
<td>800</td>
<td></td>
</tr>
<tr>
<td>Limestone aquifer</td>
<td>2.3</td>
<td>6,500</td>
<td></td>
</tr>
<tr>
<td>Sandstone aquifer</td>
<td>1.4</td>
<td>17,000</td>
<td></td>
</tr>
<tr>
<td>Alluvial aquifer</td>
<td>0.6</td>
<td>150</td>
<td></td>
</tr>
<tr>
<td>Limestone aquifer</td>
<td>2.3</td>
<td>3,500</td>
<td></td>
</tr>
<tr>
<td>Chalk</td>
<td>1.7</td>
<td>7,500</td>
<td></td>
</tr>
<tr>
<td>Alluvial aquifer</td>
<td>0.8</td>
<td>820</td>
<td></td>
</tr>
<tr>
<td>Sandstone aquifer</td>
<td>0.6</td>
<td>45,000</td>
<td></td>
</tr>
</tbody>
</table>

In groundwater modeling where parameter values cannot be measured at all locations, geostatistics provides methods that can predict values at unmeasured locations. It allows the uncertainty in the spatial distribution of the property to be factored in to the predicted values. If the property (such as hydraulic conductivity) is sampled at various locations, and the spatial variability of the samples analysed, patterns can be detected that can help in predicting the parameter value at unsampled locations. This divides parameter into two components: a deterministic one that varies smoothly in space and an erratic one (Kolterman and Gorelick 1996). The deterministic component allows for a statement to be made about the likely range of values to which the unsampled value belongs – i.e. in an area with high hydraulic conductivity it is more likely that the unsampled hydraulic conductivity values will also be high. The erratic component
is the one that prevents one from making accurate predictions. Geostatistics provides models for this type of phenomena, using random space functions (RSF) to model aquifer properties (Kolterman and Gorelick 1996). When this method is used, the resulting capture zone will also be a RSF. Thus uncertainty in the input of the analysis can be represented in the output of the analysis. This gives a more honest representation of the capture zone which explicitly identifies and quantifies the uncertainty that exists about its location.

2.5.5 The natural-log normal distribution

A distribution is natural-log normally distributed when the natural log of the set of the random variables in that distribution is normally distributed. Like the normal distribution, the natural-log normal distribution is also defined with the mean, \( \mu \) and the variance, \( \sigma^2 \).

Previous studies of the spatial structure of selected aquifers suggested that hydraulic conductivity values are natural-log-normally distributed (e.g. Hoeksema and Kitanidis 1985, van Leeuwen 2000). Mathematically stated, the function:

\[
Y = \ln X
\]

Equation 2-25

is normally distributed, where \( X \) can be hydraulic conductivity, \( K \). The natural-log normal distribution can be derived from the normal distribution and reads:

\[
f_X(x) = \frac{1}{x \sigma_Y \sqrt{2\pi}} \exp \left[ - \frac{(\ln x - \mu_Y)^2}{2 \sigma_Y^2} \right]
\]

Equation 2-26

where \( \mu_Y \) and \( \sigma_Y \) are the mean and standard deviation of \( Y \). The mathematical expectation or arithmetic mean of \( X \) is (van Leeuwen 2000):
\[ X_A = \mu_X = E(X) = \exp(\mu_Y + \frac{1}{2} \sigma_Y^2) \]

**Equation 2-27**

The variance of X can be written as a function of \( \mu_Y \) and \( \sigma_Y \) and is given by (van Leeuwen 2000):

\[ \sigma_X^2 = \left[ \exp(\sigma_Y^2) - 1 \right] \left[ \exp(2\mu_Y + \sigma_Y^2) \right] \]

**Equation 2-28**

The cumulative natural-log normal distribution function is given by:

\[ F_X(x) = \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{\ln x - \mu_Y}{\sigma_Y \sqrt{2}} \right) \right] \]

**Equation 2-29**

The natural-log normal distribution is dependent on the mean, \( \mu \) and the variance, \( \sigma^2 \). As the variance increases, the distribution becomes more skewed (to the left). The mean and variance in hydraulic conductivity (\( \mu_X \) and \( \sigma_X^2 \)) in Equation 2-25 to Equation 2-27 are determined by the input parameters \( \mu_Y \) and \( \sigma_Y^2 \). For random field generation based on this distribution, \( \mu_Y \) and \( \sigma_Y^2 \) must be specified (see chapter 3). Typical values for the variance, \( \sigma_Y^2 \) are shown in Table 2-3 in the previous section. \( \mu_Y \) and \( \sigma_Y^2 \) can be calculated from spatial data obtained in field measurements.

### 2.5.6 Limitations of using the natural-log normal distribution

Representing heterogeneity in hydraulic conductivity through the natural log-normal distribution is often more accurate than using a homogeneous assumption. Nevertheless, there are downfalls in using statistical methods to represent reality. Some of these weaknesses are addressed by Koltermann and Gorelick (1996). They commented that the mechanism by which sedimentary deposits form are not addressed by spatial statistical estimations used to reproduce sedimentary geometry. Even though it may result in geologically unreasonable values being interpolated, Koltermann and Gorelick (1996) still concluded that patterns of aquifer heterogeneity can be successfully reproduced using spatial statistical estimations.
Abrupt transitions or discontinuities of hydraulic properties such as faults along different rock types are not captured by the natural-log normal distribution assumption. Some cases of complex spatial variability, such as buried channels formed by meandering streams, may also not be accurately represented by these methods (Koltermann and Gorelick 1996). Care should be taken when applying this spatial distribution estimation method in practical applications in ensuring the absence of abrupt transitions and complex spatial variability in hydraulic properties.

### 2.6 Stochastic Modelling for uncertainty

The uncertainty associated with a numerical groundwater model derives from the conceptual model itself or with the data and parameters associated with the various components of the model. Some model parameters such as hydraulic conductivity and recharge are particularly prone to uncertainty, as described in the last section. Calibrating a model to a rich set of observation data (monitoring wells, stream flows, etc.) may reduce this uncertainty somewhat. However, calibration data are often scarce and even well-calibrated models have a high level of uncertainty.

One method for dealing with uncertainty is to utilize a stochastic modelling approach. With a deterministic approach (non-stochastic approach), a single model is developed that represents the best estimate of the real system being simulated. This model is used to make predictions. With a stochastic approach, a set of models is constructed where each model in the set is thought to be equally probable. Each model is then used to make the prediction or simulate a given scenario and the results are used to estimate a probability or risk that a certain outcome will occur. While this approach still relies on the underlying model assumptions to generate the initial parameter estimates, it more honestly reflects the uncertainty associated with modelling. A more detailed discussion on stochastic methodologies can be found in section 2.7.2.

#### 2.6.1 Monte Carlo (MC) simulation

The use of a large number of equally probable representations of the system to approximate stochastic processes, such as the geology is known as the Monte Carlo (MC) method. A flow equation for each representation is solved using standard numerical methods, and a statistical analysis is done for the results of all the
representations (Zhang 2002). This method is the most common approach to solving stochastic flow equations.

Monte Carlos simulations are based on statistical sampling, which originated in the late eighteenth century (Zhang 2002). Until the relatively recent introduction of electronic computers, this method was not widely applied due to the labour and time required.

With the Monte Carlo method, the user specifies a mean and a standard deviation (or variance). A minimum and maximum value can also be specified for the required parameter. In addition, the parameter can be specified as linear, normal or log-normally distributed. In this thesis, hydraulic conductivity is assumed to follow a natural-log normal distribution as discussed in section 2.5.5. The number of simulations is then specified. Each simulation is random but follows the specified distribution using the mean, standard deviation (or variance), maximum value and minimum value (if specified).

2.6.2 Weaknesses of the Monte Carlo method

The major drawback of the Monte Carlo method is its high computational requirements due to the need to solve many realisations. The quality of the simulations is also important as Zhang (2002) found that different sets of Monte Carlo simulations may produce significantly different results for the same problem.

Zhang (2002) also discusses two types of errors associated with Monte Carlo simulations. The first type of error, statistical error, is produced by the method used to generate the realisations and the number of realisations. The second type of error, numerical error, is dependant on the numerical method and solver used, as well as the spatial and temporal discretisation. Smaller spatial discretisation is generally required for larger spatial variability, but is limited by available computational power and the ability of the numerical methods limits this. The balance between computational effort, spatial discretisation and the associated numerical error used for this thesis is discussed in chapter three.
2.7 Past studies in numerical simulations of capture zones

Before presenting the stochastic approach used in this thesis in the next chapter, this section gives a brief summary of the deterministic and stochastic approaches that past studies have used. Both deterministic and stochastic methodologies consist of similar, consecutive steps. Moreover, a sophisticated version of the deterministic methodology exists which adopts techniques from geostatistics and which has a sequence of steps which closely resembles the stochastic approach.

2.7.1 Deterministic methodology

The flow chart of the simplest deterministic methodology, using parameterisation of hydraulic conductivity, is shown on the left hand side of in Figure 2-6 (van Leeuwen 2000). Firstly, one value of hydraulic conductivity is obtained (for example from a pumping test) and assigned to all grid nodes of the grid representing the groundwater flow domain. This homogeneous hydraulic conductivity field is then used in a steady state groundwater flow simulation in order to calculate the distribution of the hydraulic heads. Thirdly, the head field is used in conjunction with the hydraulic conductivity field to determine the average groundwater flow velocities in all grid nodes of the flow domain. These are then used in a particle tracking analysis to calculate flow paths and travel times from virtual particles released at all grid nodes of the flow domain. Finally, the flow paths and travel times are used to delineate the boundaries of the capture zones.
Figure 2-6: Methodologies of deterministic and stochastic approaches - adopted from van Leeuwen (2000).

This method produces a deterministic solution with a homogeneous field. Traditionally, this method has always been used to determine the capture zone and its advantage lies in its simplicity and the ability to give a quick impression. It does not take into account of heterogeneity or uncertainty. Studies have shown that deterministic solutions generate large errors in the results due to incorrect parameterisation of aquifer properties (Bhatt 1993). The results in this thesis will investigate the level of deviation of the heterogeneous capture zones from the traditional homogeneous one.

A slightly more complex deterministic method consists of taking more than one measurement of hydraulic conductivity and dividing the groundwater flow domain into different zones of equal hydraulic conductivity. The subsequent steps are similar to those described above, the only difference being that the hydraulic conductivity field is now in homogeneous blocks instead of completely homogeneous. The steps
are shown second from the left in Figure 2-6. An example of this technique can be found in the study carried out by Rahbeh (1999). In this study, heterogeneity was represented by 10 separate blocks of hydraulic conductivity values dependant on measurements taken. Although this method is a better representation in comparison to a homogeneous field, blocks of soil with sudden changes of hydraulic conductivity do not accurately represent properties of real world aquifers.

The most sophisticated parameterisation consists of kriging several hydraulic conductivity measurements in order to obtain an estimated map of hydraulic conductivity values. The consecutive steps in this methodology are diagrammatically represented in Figure 2-6, third from the left. Kriging is an estimation procedure using known values and a semivariogram (such as the natural-log natural distribution) to determine unknown values (Journel and Huijbregts 1978). Firstly, a limited number of hydraulic conductivity values are measured. Secondly, the measured values are used in a structural analysis in order to estimate the semivariogram, or spatial correlation structure of the hydraulic conductivity field. The variogram, together with the mean of the measurement values, is then used to perform kriging. An estimate is made of the values at all unmeasured locations on the grid. The thus obtained hydraulic conductivity field, consisting of the measured values at the measurement locations and the kriged values at the unmeasured locations, is then used in the same manner as in the previous methodologies, resulting in a deterministic capture zone. Although this method produces one deterministic solution, it produces a heterogeneous field based on an assumed distribution of the hydraulic conductivity and spatial correlation structure.

2.7.2 Stochastic methodology

The important disadvantage of the deterministic approaches is that the uncertainty resulting from hydraulic conductivity heterogeneity is not taken into account. The general idea to stochastic modelling of groundwater flow involves viewing the porous medium as a realisation of a random function. The uncertain parameter is described as a random process with known spatial statistical properties (such as the variance and correlation length) and the flow equation is solved in order to determine the distribution of the hydraulic head, which will now also be a random function. The problem to be solved is the inference of the unknown spatial statistical properties of
the latter function, i.e. its spatial probability distribution. Only in relatively simple flow situations can this be done analytically (van Leeuwen 2000).

Using stochastic simulations for capture zone analysis is a relatively new concept in literature. Limited studies have been carried out using this method in combination with a heterogeneous field. This is due to the large computational times and higher complex models required. This may not be a continual trend as computers carrying out numerical simulations have become much more efficient over recent years.

For stochastic capture zone analysis, the consecutive steps of the methodology are shown on the right hand side in Figure 2-6. A comparison with the methodology used for deterministic capture zone analysis shows that the steps taken are similar. The first two steps of measuring the hydraulic conductivity at different locations and estimating the spatial statistical properties of the field are the same as for the deterministic delineation (third from the left in Figure 2-6). In this study, no actual field data was used but the fields were conditioned using statistical parameters of the mean \(10^{-11}\text{m.s}\), variance (3 for the standard case) and correlation length (20m for the standard case) of hydraulic conductivity. After this, the third step is a stochastic simulation of one hydraulic conductivity field with the same spatial statistical properties as the set of measured (or assumed) values. The simulated hydraulic conductivity field is then used to delineate one capture zone in the same manner as in the deterministic methodologies. The procedure continues with a Monte Carlo analysis, repeating steps 3 to 5 a number of times. Each repetition gives a random heterogeneous hydraulic conductivity field based on the same statistical parameters followed by a deterministic capture zone. Each of these capture zones are treated as equally probable and combined to create a capture zone probability distribution (capd) from statistical analysis. This approach uses a heterogeneous field and at the same time gives a description of the level of uncertainty by using a capd.

Riva et al. (1999) studied the influence of conductivity heterogeneity on the location of capture zones in a Monte Carlo setup, but with a zero background flow. An empirical, stochastic expression for the location of the circle-shaped capture zone was found.
Franzetti and Guadagnini (1996) and Guadagnini and Franzetti (1999) studied the influence of hydraulic conductivity heterogeneity on the location of well catchments and capture zones with a uniform background flow. They performed a series of unconditional Monte Carlo simulations with various degrees of domain heterogeneity, that is, hydraulic conductivity variance. Random hydraulic conductivity fields were generated using the Fast Fourier Transform algorithm and particles were released at all nodes of the grid. The results were treated statistically to obtain capture zone probability distributions. They found an empirical, stochastic expression for the location of the capture zone and the well catchment, based on an analytical solution for capture zones in homogeneous porous media by Bear and Jacobs (1965).

The spatial stochastic approach for determining capture zones was also adopted by Varljen and Shafer (1991). MC simulations were performed with hydraulic conductivity fields generated using a Turning Bands algorithm (Montaglou and Wilson 1982) and they subsequently conditioned them on hydraulic conductivity data using a kriging technique. Reverse particle tracking was applied in order to determine the 1-year and 10-year capture zones. They determined an average capture zone and corresponding 95 percent confidence limits. They then defined the region between the upper and lower confidence limit capture zones as the zone of uncertainty. A demonstration was conducted, using one randomly generated hydraulic conductivity field as the reference, “true” field. This then provided the opportunity to generate a reference capture zone, based on all the “true” data from the reference field. The 25 conditioning conductivity values were sampled from the reference field at locations scattered around and upstream of the well. They concluded that the zone of uncertainty about a time-related capture zone is influenced by both natural hydrological conditions and the pattern used for sampling aquifer properties. Therefore, wise selection of sample locations could offset increases in uncertainty that have been shown to occur as a result of hydrological conditions (that is, the regional gradient).

Van Leeuwen and te Stroet (1998) studied the effects of the statistical parameters of transmissivity variation (the variance and correlation structure) on the capd for a fully confined and a leaky-confined aquifer. They used unconditional simulations and found that the capd to be cumulative distributed for sufficiently small variance and
correlation structure values in both aquifer models. Uncertainty in the capture zone increases as time and variance increases in the fully confined aquifer case. In the leaky confined case, uncertainty is more dependent on the correlation structure in comparison to the fully confined case. Van Leeuwen (2000) further used a conditioned stochastic methodology to determine capds in Wierden (Netherlands). In his study, van Leeuwen concluded that the stochastically determined capture zones revealed uncertainty while deterministic capture zones obscure it. Stochastic estimation preserves the discontinuous character of clay layers while there are large potential risks associated with using a deterministic approach.

Past stochastic studies have focused solely on the effects of the variance and correlation structure of the heterogeneity on the extent of uncertainty about the location of a capture zone. There is a gap between the studies carried out under a homogeneous assumption and those using heterogeneous fields. In homogeneous studies, the capture zone is determined by the aquifer and well properties such as the hydraulic gradient, the well pumping rate and the hydraulic conductivity of the soil. Past studies of capture zones using heterogeneous conditions fail to acknowledge that the fundamental aquifer and well properties that determine the homogeneous capture zone may cause changes in the behaviour of uncertainty. There are also little documentation of the effects of anisotropy and the spacing between two wells on the level of uncertainty in heterogeneous formations.
Chapter 3

Methodology
3 Methodology

The stochastic simulations carried out in this thesis follows the general layout outlined in Section 2.7.2. Although many of the aquifer and well properties are varied between simulations, they follow similar steps. This chapter will firstly give a brief background on the programs used for the simulations. It will then follow with a detailed description of the numerical methodology used for obtaining estimates of the capture zone probability distributions.

3.1 MODFLOW

Modflow is the US Geological Survey modular finite-difference groundwater flow model. It is a computer model that simulates saturated three-dimensional groundwater flow through a porous medium, including unconfined, confining and confined layers (Harbaugh et al. 2000). It numerically solves the three-dimensional groundwater flow equations using the finite-difference method. Transient and steady-state flow can be simulated, and a variety of processes can be included in the model, such as rivers, wells, and recharge (Harbaugh and McDonald 1996).

The design concepts of Modflow will be discussed in this section. The aspects of the model with direct relevance to the understanding of the numerical methods used in this study will be briefly described.

3.1.1 Modular structure

Modflow’s modular structure is divided in several different ways – processes, packages, procedures and modules. Similar program functions are grouped together, and computational and hydrologic options are constructed so that they are independent of other options (McDonald and Harbaugh 1988). The program is divided into packages from a user’s perspective. Each individual package deals with an aspect of the simulation. For example, the wells package simulates the effect of wells (McDonald and Harbaugh 1988). A package may also consist of a solution method used to solve the simultaneous equations resulting from the finite-difference method. The remainder of the code not included in the hydrologic or solution packages form the Basic Package, providing overall program control (Harbaugh et al. 2000).
From a programmer’s perspective, the program can be divided into pieces called procedures (Harbaugh et al. 2000). The new modularization entity of processes was introduced in MODFLOW-2000. A process is a part of the code that uses a specified numerical method to solve a fundamental equation, such as the Groundwater Flow Process (Harbaugh et al. 2000).

The program code can be divided into smaller pieces that are called modules. A module consists of the program code within a single procedure for a single package. The code for a package is contained in all the modules that correspond to that package. Likewise, the modules for a procedure or a process contain all the code that correspond to that procedure or process (Harbaugh et al. 2000).

### 3.1.2 General model discretisation in Modflow

#### 3.1.2.1 Spatial discretisation

Modflow’s finite difference grid must be rectangular horizontally, but can be distorted vertically (Harbaugh et al. 2000). For each individual cell, the complete geometry needs to be defined, as certain processes such as transport modelling may potentially need this information (Harbaugh et al. 2000). Rows of the Cartesian grid are numbered beginning from the upper edge of the grid and have the denotation ‘i’. Columns, labelled ‘j’, are numbered starting from the left side of the grid. The numbering of layers, denoted ‘k’, begin from the top layer downwards. The top elevation of the top layer and the bottom elevation of every layer need to be defined (Harbaugh et al. 2000).
3.1.2.2 Temporal discretisation

Modflow can simulate steady state or transient conditions. Time steps are the main component of time discretisation in MODFLOW. Time steps are grouped into stress periods. Input data, such as the total length of time, the number of time steps and the multiplier for the length of successive time steps, have to be entered for every stress period (Harbaugh et al. 2000).

A single time step is required for steady-state stress periods in MODFLOW (Harbaugh et al. 2000). Consistent units of length and time must be used for the input data, as the groundwater flow process of Modflow formulates the groundwater flow equation without using any specific units (Harbaugh et al. 2000). This particular process is discussed in the next section.

3.1.3 Groundwater flow process

The groundwater flow process solves the groundwater flow equation using the finite difference method (Harbaugh et al. 2000). The partial-differentiation equation of groundwater flow given in Section 2.3.2 (Equation 2-12) is used in Modflow (McDonald and Harbaugh 1988). When boundary and initial conditions are included and the principal axes of hydraulic conductivity are aligned with the coordinate
directions, the equation describes transient three-dimensional groundwater flow in a heterogeneous and anisotropic medium (Harbaugh et al. 2000).

This process solves the equation using the finite-difference method. The aquifer system is divided into a grid of cells. Each cell contains a single point, called a node, where the hydraulic head is calculated (Harbaugh et al. 2000). The finite-difference equation for a cell is shown in Equation 3-1 (McDonald and Harbaugh 1988):

\[
\begin{align*}
CR_{i,j+1/2,k} \left( h_{i,j+1/2,k}^m - h_{i,j,k}^m \right) + CR_{i,j+1/2,k} \left( h_{i,j+1,k}^m - h_{i,j,k}^m \right) + CC_{i,j+1/2,k} \left( h_{i,j,k}^m - h_{i,j+1,k}^m \right) + CC_{i-1/2,j,k} \left( h_{i-1/2,j,k}^m - h_{i,j,k}^m \right) + CC_{i+1/2,j,k} \left( h_{i+1/2,j,k}^m - h_{i,j,k}^m \right) + CV_{i,j,k-1/2} \left( h_{i,j,k}^m - h_{i,j,k-1}^m \right) + CV_{i,j+1,k-1/2} \left( h_{i,j,k}^m - h_{i,j+1}^m \right) + P_{i,j,k} h_{i,j,k}^m + Q_{i,j,k} = SS_{i,j,k} \left( DLR_j \times DELC_i \times THICK_{i,j,k} \right) \frac{h_{i,j,k}^m - h_{i,j,k}^{m-1}}{t_m^m - t_m^{m-1}}
\end{align*}
\]

Equation 3-1

where \( h_{i,j,k}^m \) is the head at cell \( i,j,k \) at time step \( m \) [L]; \( CV, CR \) and \( CC \) are the hydraulic conductances between node \( i,j,k \) and adjacent the adjacent node \([L^2T^{-1}]\); \( P_{i,j,k} \) is the sum of coefficients of head from the source and sink terms \([L^2T^{-1}]\); \( Q_{i,j,k} \) is the sum of constants from the source and sink terms \([L^3T^{-1}]\); \( SS_{i,j,k} \) is the specific storage \([L^{-1}]\); \( DLR_j \) is the cell width of column \( j \) in all rows \([L]\); \( DELC_i \) is the cell width of row \( i \) in all columns \([L]\); \( THICK_{i,j,k} \) is the vertical thickness of cell \( i,j,k \) \([L]\); and \( t_m \) is the time at time step \( m \) \([T]\).

The storage term in the groundwater flow equation (Equation 2-12) is the only component of the equation that depends on the length of time. In steady-state conditions, such as the simulations carried out in this thesis, this term is set to zero (Equation 2-13). The subscript notation ‘1/2’ is used to denote hydraulic conductance between nodes, rather than conductances within a cell. For example, \( CR_{i,j+1/2,k} \) is the conductance between nodes \( i,j,k \) and \( i,j+1,k \) (Harbaugh et al. 2000).

When Equation 3-1 is applied to all cells, a set of simultaneous equations is produced. These equations are solved for head at the nodes where this is required. The user defines whether head should be calculated for each cell (called a variable-head cell),
water cannot flow through a cell (no-flow cell), or that the head’s specified value remains constant (constant-head cell). Equation 3-1 is modified to Equation 3-2 below when solved by computer (Harbaugh et al. 2000):

\[
CV_{i,j,k} \frac{h_{i,j,k-1} - h_{i,j,k}}{\frac{1}{2} h_{i,j,k}} + CC_{i,j,k} \frac{h_{i,j,k} - h_{i,j+1,k}}{\frac{1}{2} h_{i,j,k}} + CR_{i,j,k} \frac{h_{i,j,k} - h_{i,j,k-1}}{\frac{1}{2} h_{i,j,k}} + \left( -CV_{i,j,k} \frac{h_{i,j,k} - h_{i,j,k-1}}{\frac{1}{2} h_{i,j,k}} - CR_{i,j,k} \frac{h_{i,j,k} - h_{i,j,k-1}}{\frac{1}{2} h_{i,j,k}} - HCOF_{i,j,k} h_{i,j,k} + CR_{i,j,k} \frac{h_{i,j,k} - h_{i,j+1,k}}{\frac{1}{2} h_{i,j,k}} + CC_{i,j,k} \frac{h_{i,j,k} - h_{i,j+1,k}}{\frac{1}{2} h_{i,j,k}} \right)
\]

Equation 3-2

Equation 3-2 above applies for time step m. The term HCOF\(_{i,j,k}\) includes P\(_{i,j,k}\) and the part of the storage term that includes the head in the current time step (now negative). The right hand side of the equation includes Q (now negative) and the part of the storage term that is multiplied by the head at time step m-1 (Harbaugh et al. 2000).

CV, CR and CC coefficients and the storage related parts of HCOF and RHS are calculated by the internal-flow package (Harbaugh et al. 2000). The internal-flow package of the Layer-Property Flow (LPF) Package was used for simulations in this thesis. Components of this package relevant to this study are discussed in the next section. Source-sink packages, such as the well package, are also used to contribute source or sink terms to the groundwater flow equation. Sources are defined as positive sinks (Harbaugh et al. 2000).

### 3.1.4 The Layer-Property Flow (LPF) package

The Layer-Property Flow (LPF) is an alternative to the Block-Centered Flow (BCF) Package, another internal-flow package, which performs the same function and is conceptually similar. The two packages differ mainly in the input data that the user provides. In the LPF package, all of the input data defining hydraulic properties are independent of the dimensions of the cell, unlike in the BCF package. For example, transmissivity is entered by the user for the BCF package in some situations, but is never entered in the LPF package (Harbaugh et al. 2000).
A node is assumed to be located at the centre of each model cell. Conductance is defined for a direction of flow and a prism of material, and is described by Equation 3-3 below (Harbaugh et al. 2000).

\[ C = \frac{KA}{L} \]

*Equation 3-3*

where \( C \) is the conductance \([L^2 T^{-1}]\), \( K \) is the hydraulic conductivity in the direction of flow \([LT^{-1}]\), \( A \) is the cross-sectional area perpendicular to the flow \([L^2]\) and \( L \) is the length of the flow path \([L]\).

Darcy’s Law from SECTION 2.3.1 (Equation 2-9) can be written in the form shown below (Harbaugh et al. 2000).

\[ Q = C(h_2 - h_1) \]

*Equation 3-4*

The finite-difference equations of Modflow use equivalent conductances between nodes of neighbouring cells, also known as branch conductances. The equivalent conductance can be calculated using Equation 3-5, assuming the conductances are arranged in series (Harbaugh et al. 2000).

\[ C = \frac{C_1 C_2}{C_1 + C_2} \]

*Equation 3-5*

Since simulations in this thesis are carried out in two dimensions, only horizontal conductance is of direct relevance. The horizontal conductance terms, CR and CC, of the groundwater flow equation (Equation 3-2) are calculated between adjacent horizontal nodes. The CR term specifies the conductance between two nodes in the same row, and CC is the conductance between adjacent nodes in the same column (Harbaugh et al. 2000).
Horizontal conductance can be calculated in three different ways in the LPF package. Each method makes different assumptions about how the system varies from cell to cell. The harmonic mean method, used in this thesis, makes the assumption that transmissivity (hydraulic conductivity multiplied by thickness) is constant within a cell, and changes in the boundary between any two cells (Harbaugh et al. 2000).

### 3.1.5 Sources and sinks – the well package

The Well Package simulates wells that recharge or discharge water from an aquifer. The rate at which each well injects or removes water from the aquifer, denoted Q, during every stress period is specified by the user. It is independent of both the cell area and the head in the cell. Positive values of Q indicate a recharging well, and well discharge is denoted by negative values of Q (McDonald and Harbaugh 1988).

When a well is placed at a certain cell, the value of Q is subtracted from the right hand side term of Equation 3-1 for each iteration step for that particular cell. If there is more than one well in a cell, the total discharge or recharge from the wells is found and subtracted from the RHS term (McDonald and Harbaugh 1988).

### 3.2 Random field generation and FGEN

Random field generators are used to generate fields of stochastic properties that have known statistical attributes. An example is hydraulic conductivity, which can be assumed to be natural-log normally distributed. Randomly generated fields cannot replace actual measurements, as they are only as representative of reality as the statistical or geological model that they are based on (Robin et al. 1993). The generated random fields are equally probable representations of a formation, and any single field will usually not reproduce the input statistics used to generate the field.

Random field generators have been used in the assessment of the sensitivity of the natural system to extreme realisation scenarios (Zhang 2002). They have also been used to estimate measurements and forecast uncertainties due to geological variability, and to interpolate between observations (Robin et al. 1993). Random field generators have been used to verify stochastic-analytical theories of groundwater flow and solute
transport through coupling with numerical simulators. Synthetic random fields have been used in investigating the effects of spatially varying aquifer properties on the mean transport of contaminants (Robin et al. 1993).

There are various methods used for random field generation, including, but not limited to, the turning bands method, matrix decomposition, Gaussian sequential simulations and spectral domain fast Fourier methods (Koltermann and Gorelick 1996; Zhang 2002). A computer algorithm, referred to as FGEN, was used in this study. It is capable of generating three dimensional random fields, based on the direct Fourier transform method (Robin et al. 1993). Only two dimensional fields were generated though, for the purpose of this thesis.

In generating a random field, the dimensions with a number of points corresponding to a power of two are transformed by FGEN using the fast Fourier transform, and the others with a regular Fourier transform algorithm. The fast Fourier transform is more computationally efficient and minimises round-off error (Robin et al. 1993). It is therefore much more efficient to specify field dimensions with a power of two. The generated fields lie on a three-dimensional grid with constant spacing between points in any given direction (Robin et al. 1993). The grid spacing can vary between directions. Fields generated are circularly periodic, but this can be managed by generating fields with larger dimensions than required and truncating the fields. Grid dimensions and grid spacings need to be adjusted to minimise the spectral discretisation and truncation errors. Anisotropy in any direction can be handled by the algorithm (Robin et al. 1993).

### 3.3 Parameterisation of hydraulic conductivity

In this thesis, heterogeneous hydraulic conductivity values are assumed to follow a natural-log normal distribution with defined statistical mean and variance values (as discussed in Section 2.5.5). Since there is no conditioning data used, a mean hydraulic conductivity value of $10^{-11}$ m/s was used – representing average medium sand soil.

In past studies, the variance of the natural-log normal distributed hydraulic conductivity was found to vary in the range of approximately 0.5 to 5 (see Section...
2.5.4, Table 2-3). The variance represents the variability about the mean and is shown in Equation 2-28 in Section 2.5.3. The variance in the natural log-normal distribution determines the spread and skew of the graph.

![Graphical representation of the natural-log normal distribution with changing standard deviation (square root of the variance)](image1)

**Figure 3-2:** Graphical representation of the natural-log normal distribution with changing standard deviation (square root of the variance)

![Graphical representation of the cumulative natural-log normal distribution with changing standard deviation (square root of the variance)](image2)

**Figure 3-3:** Graphical representation of the cumulative natural-log normal distribution with changing standard deviation (square root of the variance)

For hydraulic conductivity values, a higher variance represents a higher level of heterogeneity in the soil. The variance is often changed in simulations carried out in
this thesis to observe the effects of increasing heterogeneity. The standard base case usually uses a variance value of 3.

The spatial persistence of the correlation between neighbouring hydraulic conductivity values can be quantified by defining a correlation length. The correlation length value represents a distance at which two points are no longer correlated. This can be used to estimate the size of generated lenses of similar hydraulic conductivities in an aquifer. As shown in see Section 2.5.4, Table 2-3, the horizontal correlation length varies from a few meters to a few thousand meters dependent on the soil type and viewing scale. In this thesis, the standard correlation length used is 20m in both the ‘i’ (x) and ‘j’ (y) directions.

3.4 Grid discretisation

Consideration on issues regarding boundary conditions and relevant process scales are important when choosing a domain size and discretisation level. In general, Davies (1987) concluded that the higher the discretisation level of the flow problem and the hydraulic conductivity field, the better the subsequent solution to the groundwater flow equation. However, higher discretisation levels require greater computational time and effort. It is therefore important to find a balance between the level of discretisation and computational time.

In capture zone analysis, the flow patterns are mostly radial. However, a Cartesian grid with uniform, square grid spacing is adopted in this thesis. A Cartesian grid with a geometric refinement of spacing towards the well - or even better, a radial grid with a geometric refinement of spacing towards the well - ensures a more accurate numerical calculation of heads in the vicinity of the well for capture zone analysis (van Leewen 2000). However, this discretisation approach is not adopted here because of the problem of assigning hydraulic conductivity values to blocks varying in size over orders of magnitude.

In order to get an accurate reproduction of the correlation structure of the hydraulic conductivity field, past studies have shown that a sufficient number of generation points per correlation scale must be chosen, i.e. the ratio of grid size to the correlation
length used. For a flow problem with a uniform mean hydraulic gradient, Ababou et al. (1989) suggested as a rule of thumb the following ratio between the grid size, \( \Delta x \) and the correlation length, \( C_L \):

\[
\frac{\Delta x}{C_L} \leq \frac{1}{1 + \sigma_K^2}
\]

**Equation 3-6**

where \( \sigma_K^2 \) is the statistical variance of hydraulic conductivity.

All simulations carried out in this thesis use a grid size of one meter. The ratio in Equation 3-6 holds for all the simulations carried out in this study – the lowest correlation length used was \( C_L = 5 \) m and the highest variance value used is five.

In stochastic groundwater flow fields, boundary conditions influence the transport properties up to a distance that increases with variance and correlation length. Previous studies have shown this effect for cases with a mean uniform gradient (e.g. Bellin et al. 1992). To avoid these effects, the size of the domain generated through FGEN is larger than the actual field used and is truncated to the required size. For large variance and correlation length values, boundary conditions may influence the capture zone and will be accounted for in the text.

In all the simulations carried out in this thesis, the grid cells used measures 500×500×1. The scale of consideration for this thesis assumes the vertical dimension is small compared to the horizontal dimension. Therefore the aquifer thickness can be averaged and represented as two-dimensional. Each node has a size of 1 m by 1 m (in the x and y directions) and the total amount of grid nodes are therefore 250 000. This is shown in Figure 3-4 below.
Figure 3-4: Dimensions of one heterogeneous field, with darker areas representing lower hydraulic conductivity values.

Figure 3-4 shows the orientation of the field in respect to North. This direction is chosen arbitrarily as a reference to make explanations and discussions easier to understand.

3.5 Boundary and initial conditions

The origin of the Cartesian coordinates in this system is located in the south-western corner as shown in Figure 3-4. No flow boundary conditions are imposed at the east and west boundaries (at x=500 and x=0). Fixed head conditions are imposed at the north and south boundaries (y=500 and y=0). This establishes a constant ratio between the domain length and the head difference between the north and south boundaries – creating an initial uniform hydraulic gradient. Constant head boundaries are established in Modflow by selecting the required cell and using the cell properties option to assign a value of −1 for IBOUND. Other grid cells remained active and were assigned a default IBOUND value of 1. For the base case, the hydraulic head at the southern boundary is set at 100m while the northern boundary is set at 95m giving a hydraulic gradient of 0.01. This value is chosen as it represents a typical background
hydraulic gradient in the porous media. Other active cells have an initial hydraulic head of 97m.

3.5.1 Extraction well

In most simulations, an extraction well is placed at the cell location x=250, y=400. The well is placed in this position to maximise the capture zone viewability, both down-gradient and up-gradient of the well. The position of the well was tested in several other positions and this location corresponded most suitably to the pumping rate used in a single well simulation. The standard pumping rate used was 0.02 m$^3$/s. Different extraction rates and well positions were tested under homogeneous hydraulic conductivity conditions. In terms of size, shape and location of the capture zone, this standard extraction rate and well position resulted in a capture zone most suitable for the chosen domain. Figure 3-5 below shows the size, shape and location of the capture zone under homogeneous conditions at steady state. This capture zone uses the standard values for hydraulic conductivity, hydraulic gradient, well position and pumping rate.

![Figure 3-5: Base case capture zone simulation under homogeneous conditions. $K=10^{-11}$ m/s (medium sand), hydraulic gradient = 0.01, well position x=250, y=400, $Q=-0.02$ m$^3$/s.](image)
3.6 Generating heterogeneous fields using FGEN

FGEN is a cross-correlated random field generator using the direct Fourier transform method and is explained in Section 3.2. The program reads conditioning data from a text input file with a `*.gen` extension. For each aquifer or well property investigated in this thesis, ten heterogeneous fields were used to generate a capture zone probability distribution. Each map was generated in FGEN while changing the random seed number. Figure 3-6 below shows two fields generated with the same spatial statistical parameters but using different random seed numbers.

![Figure 3-6: Two heterogeneous fields with the same spatial variability statistical parameters, but different random seed number. The darker areas represent lower hydraulic conductivity values.](image)

3.7 Monte Carlo methodology

For the simulations carried out in this thesis, each MC analysis comprises of ten realisations and each realisation consists of the following steps:

1. Heterogeneous hydraulic conductivity values are generated using FGEN. The field is conditioned on specified statistical parameters such as the mean, variance and correlation length. A different random seed number is used each time.
2. The generated file is modified to be readable by Modflow. The 250 000 values is then imported into Modflow and read in as hydraulic conductivity values.
3. Boundary and initial conditions for the domain created in Modflow will then be modified depending on what values are needed.
4. Modflow then uses the finite difference computer code (Section 3.1.3) to solve the groundwater flow equation (Equation 2-12) for the hydraulic heads at each individual node at steady state. A solution set is generated.

5. Forward particle tracking is then performed on the solution set using the computer code Modpath (Pollock 1994), whereby at least one particle is released at each grid cell in the domain.

6. The end points of all particles are recorded.

When ten realisations are generated (i.e. the MC analysis is repeated ten times), there will be ten solution sets. Every cell (total 250 000) will have had at least one particle released from it and its end point tracked for each realisation. For each particular cell, if the released particular reaches the extraction well then a counter for that cell is updated. After running Modpath on each of the Modflow solutions, the percentage of particles from a particular cell that are eventually captured by the well is computed and saved as the capture probability for the cell. The capture probability data set can then be contoured, creating a capture zone probability distribution.

### 3.8 Capture zone probability distribution (capd)

The capture zone probability distribution (capd) gives the probability that a conservative tracer particle released at a particular location is captured within a specified time span. In this thesis, the simulations are done in steady state so the time span is not defined. An example of a capd is shown in Figure 3-7. All probabilities are defined under steady state conditions. The isolines, defined by L$_i$ connects the locations in the capd with the same probability of capture of P = ‘i’ percent.

The zone of uncertainty is defined as the area where the probability of capture is between one and zero, i.e. between one hundred percent capture and zero percent capture. Mathematically stated, the zone of uncertainty is defined as 0 < P < 1. Since there are 10 realisations in each case, the probability of capture for each node will be a discrete value ranging from 0 to 1 in 0.1 increments.

The median isochrone, defined by the isoline L$_{50}$, is used as the preferred statistical measure of the capd’s location rather than the mean or expected isochrone. This is
because it is less sensitive to outliers, can be easily defined in all radial directions, is straightforward to calculate and is more easily understood (van Leeuwen 2000).

P10 is defined as the area where the probability of capture (P_{capture}) is higher than 10 percent. In other words, for simulations in this thesis, P10 represents areas with a probability of capture of at least 20 percent or higher.

P50 is defined as the area where the probability of capture is higher than 50 percent. In other words, for simulations in this thesis, P50 represents areas with a probability of capture of at least 60 percent or higher.

P90 is defined as the area where the probability of capture is higher than 90 percent. In other words, for simulations in this thesis, P90 represents areas with a probability of capture of 100 percent.

P10, P50 and P90 can be used to define the zones of uncertainty and quantify this level of uncertainty. P10 represents an area of low certainty while P90 represents an area with high certainty. These areas can also be used to measure the 80 percent zone spread around the median isochrone. The 80 percent zone can be defined as 0.1<P<0.9. Following a similar (but modified) calculation in van Leeuwen (2000), the spread of the capd can be measured and is defined as:

\[
S_{capd}^2 = \left[ \frac{1}{4} (P10 - P90) \right]^2
\]

Equation 3-7

The methodology used in van Leeuwen (2000) measures the spread by calculating the distance between the isolines, while the calculation in Equation 3-7 measures the areal spread. A better measurement of spread around the median isochrone can be achieved by defining a percentage zone higher than 80 percent, say 95 percent, i.e. using P2.5 - P97.5 instead of P10-P90. Since only ten MC realisations are made though, this is impossible as probability values are discrete in increments of 0.1. Nevertheless, the general behaviour of the spread of the capd should not be greatly affected.
Figure 3-7: A capd obtained using 10 MC analyses in Modflow. In a strict mathematical sense, L0 should be placed at an infinite distance from the well and L100 should be placed at the well.

### 3.9 Calculating the capture zone area

To calculate the area of a capd, the following steps were taken:

1. The data file within Modflow containing the capd details is isolated. This data file contains each grid cell number (1-250 000) and the probability of capture for that cell for the 10 MC simulations.

2. Three new files are created from this file using the data calculator in Modflow. The original capd data file is modified into P10, P50 and P90 data files. This is done by truncating values from the original capd data file, i.e. for P10 all values smaller than 0.1 (0 and 0.1) in the original file is removed and replaced by 0.

3. The new data files are modified into `.txt` format so it is readable in Matlab. Matlab is a high-level technical computing language and interactive environment for algorithm development, data visualization, data analysis, and numerical computation. Using Matlab, technical computing problems can be
solved faster than with traditional programming languages, such as C, C++, and Fortran (The MathWorks 2005).

4. A script was written up in Matlab (an ‘m-file’) to count the number of zeros in each of the data files. This number is then recorded and deducted from 250000 to obtain the capd area – in terms of the number of grid cells

After obtaining the area for P10, P50 and P90, the results were plotted on a graph. In each simulation, the data was also used to calculate the 80 percent zone and the spread around the median isochrone.

3.10 Monte Carlo convergence

The accuracy of the simulations is highly dependent on the number of Monte Carlo realisations ($N_{MC}$) used. There are several different documented studies on $N_{MC}$ and its relationship to the accuracy of stochastic numerical models. In general, higher $N_{MC}$ will give greater confidence and accuracy in the resulting solution. The only problems with using large $N_{MC}$ are its high computational requirements and demand on time. For instance using a modelling domain containing 250000 grid cells (500 by 500), a single stochastic solution using 10 $N_{MC}$ realisations requires up to 4 hours of computational processing time. This is using a modern Pentium M processing CPU with 1000 megabytes of random access memory. Using 5 $N_{MC}$ realisations for the equivalent scenario only required half this time (2 hours). It is therefore important to find a value of $N_{MC}$ where solutions produce enough convergence without having to use too many realisations.

Past studies on $N_{MC}$ and convergence have produced different results. Some authors argue that the convergence of results depend on the grid discretion size ($\Delta x$) while some argue it is dependent on the variance of hydraulic conductivity ($\sigma^2_K$). Franzetti and Guadagnini (1996) suggested that the convergence deteriorates with increasing $\sigma^2_K$ while van Leeuwen (1998) suggested that the convergence are not influenced by either $\sigma^2_K$ or $\Delta x$. Convergence of computations should depend on the modelling domain, grid discretisation and base parameters. Other differentiations that may drive the required $N_{MC}$ include the modelling conditions set, assumed parameter distribution and the desired accuracy. Following from this argument, the required convergence
rate may be unique for different experimental conditions. Also, different methods of testing the convergence will produce different results. For example Franzetti and Guadagnini (1996) tested the probability of capture for a cell in the same location in the domain while van Leeuwen (1998) carried out the test at varying locations.

Therefore, for the purposes of this study, a convergence test was carried out to determine the $N_{\text{MC}}$ value that showed sufficient convergence of the results. Since the most important factor in this thesis is the capture area of certainty, the P90 area (which has $P_{\text{capture}}=1$) was used to test the convergence. This was also based on the hypothesis that the area with $P_{\text{capture}}=1$ behaves more erratically in heterogeneous formations compared to lower $P_{\text{capture}}$ values, as $P_{\text{capture}}=1$ represents the area with the highest certainty. Also, since Franzetti and Guadagnini (1996) suggested that convergence deteriorates with higher $\sigma^2_K$ values, the convergence computations used $\sigma^2_K=5$. This is the highest $\sigma^2_K$ value used in the simulations within this thesis.

Different numbers of realisations were used to generate a stochastic capture zone probability distribution (capd). The base parameters used were $\Delta x=1\text{m}$, $\sigma^2_K=5$, $C_L=20\text{m}$, $Q=-0.02\text{m}^3/\text{s}$, $\nabla h=0.01$ and $\mu_K=10^{-11}\text{m/s}$. The layout of the model is the same as that described in the previous sections. The results of the convergence are shown in Figure 3-8.

![Figure 3-8: Behaviour of the capture area $P=1$ showing the convergence of $N_{\text{MC}}$ realisations.](image-url)
From the results of the convergence test, it can be seen that the area with $P_{\text{capture}}=1$ is decreases as $N_{MC}$ increases. This indicates the number of grid cells with 100 percent capture is decreasing. The fluctuation of the graph stabilises around $N_{MC}=10$ as seen by the stabilisation in the decrease. When $N_{MC}$ is increased to 15, the area of P90 does not change significantly. Even though the accuracy of convergence of $P_{\text{capture}}=1$ increases as $N_{MC}$ increases, the results suggest that $N_{MC}=10$ is sufficient to obtain an estimate of the $P_{\text{capture}}=1$ area. For the simulations presented in this thesis, $N_{MC}=10$ was adopted.
Chapter 4

Results & Discussion
4 Results and discussion

Using the methodology presented in chapter 3, random heterogeneous fields were used in Monte Carlo analyses to obtain capture zone probability distributions (capd). The results presented in this chapter investigate the capds while changing controlled aquifer or well properties. Of particular interest is the behaviour of P10, P50 and P90 and their influence on the spread of the cap around the median isochrone. This will quantify the change in the level of uncertainty associated with varying particular aquifer and well properties. A comparison will then be made to the relevant homogeneous capture zone when appropriate. A qualitative and quantitative description of the relationship between the changing parameter, the capture zone and the level of uncertainty will be then be given. All simulations were carried out in a confined aquifer at steady state.

The first section presents the results of the effects of varying aquifer properties in the porous media on the behaviour of uncertainty in the resulting capture zone. Aquifer properties that are studied include the variance of hydraulic conductivity \( \sigma_k^2 \), the correlation length of hydraulic conductivity \( C_L \) in meters, anisotropic conditions in the soil \( (C_{LX}:C_{LY}) \) and the background hydraulic gradient \( \nabla h \). The second section presents the results for changing well properties that include the well extraction rate \( Q \) in cubic meters per second, the parallel spacing between two wells and the perpendicular spacing between two wells (both in meters). The units used for the parameters will remain constant throughout this section and may be omitted for convenience.

4.1 Variance of hydraulic conductivity

The aim in this simulation is to quantify the effects of the statistical variance on the capd. The main focus is to determine a general relationship between increasing variance of hydraulic conductivity \( \sigma_k^2 \) and the resulting uncertainty within the capture zone. The influence of the variance on the size, shape and location of the resulting capture zone will be quantified by analysing the results.
Different values for the variance of hydraulic conductivity were used for and they ranged from one to five ($\sigma^2_K = 1, 2, 3, 4, 5$). 10 MC simulations were carried out for each variance value resulting in a total of 50 different heterogeneous fields (10 for each variance value), 50 deterministic solutions and 5 stochastic capds.

Following the model discretisation outlined in chapter 3, all other parameters were kept constant at their standard values, i.e. $C_L = 20\, \text{m}$, $Q = -0.02\, \text{m}^3/\text{s}$, $\mu_K = 10^{-11}\, \text{m/s}$, $\nabla h = 0.01$ and a single extraction well is located at $x=250$, $y=400$.

### 4.1.1 Homogeneous, deterministic solution

In a homogeneous case, $\sigma^2_K = 0$. The problem then reduces to a deterministic one and is described by analytical solutions in Equation 2-17 in chapter 2. The resulting capture zone at steady state for this domain is shown in Figure 3-5 in chapter 3.

### 4.1.2 Heterogeneous, deterministic solutions

For each the variance values of $\sigma^2_K = 1, 2, 3, 4$ and 5, ten heterogeneous fields were created. Figure 4-1 shows one particular field of the 10 used for stochastic analysis for $\sigma^2_K = 1, 2, 4$ and 5.
Figure 4-1: One of the random ten heterogeneous fields with $\sigma_K^2=1$ (top left), 2 (top right), 3 (bottom left) and 4 (bottom right). Darker areas represent lower hydraulic conductivity.

Figure 4-1 shows that as $\sigma_K^2$ increases the field becomes more heterogeneous, displaying higher quantities of extreme hydraulic conductivity values. When $\sigma_K^2=1$, the field is evenly shaded in comparison $\sigma_K^2=5$.

Solving each individual field for the hydraulic head at each node generates a deterministic solution under heterogeneous conditions (as explained in Section 2.7.1). The resulting deterministic solutions for Figure 4-1 are shown in Figure 4-2.
The green contours in Figure 4-2 represent areas of equal hydraulic head. Particles were released at the well (using Modpath) and the results from backward particle tracking are shown by the blue lines. Although forward tracking is used for the stochastic simulations (see Section 2.4.1.2 for the difference between forward and backward tracking), backward tracking was used here to create a fast and simple estimation of the shape of the resulting capture zone. From Figure 4-2, it can be seen that blue particle lines for low $\sigma^2_K$ values closer resemble the capture zone derived from a homogeneous assumptions (Figure 3-5). As $\sigma^2_K$ is increased, the size and shape of the capture zone begin to divert away from the homogeneous assumption. This becomes more obvious as the distance from the well increases.
4.1.3 Heterogeneous, stochastic results

The results of combining 10 MC simulations with different $\sigma_K^2$ values are shown in Figure 4-3 and Figure 4-4 as a capd.

Figure 4-3: Capture zone probability distribution obtained for $\sigma_K^2=1$
Figure 4-4: Capd plots for $\sigma^2_K = 2$ (top left), 3 (top right), 4 (bottom left) and 5 (bottom right)

Uncertainty in the isolines (bordering the isochrones of equal probability) results in the uncertainty in the boundaries of the capture zone. It can be seen from Figure 4-3 and Figure 4-4 how an increase in $\sigma^2_K$ results in the expansion of the zone of uncertainty (area between $P=1$ and $P=0.1$). Without analysing the exact area of each probability distribution, the capd already show an obvious increase in uncertainty in defining the shape of the capture zone for higher $\sigma^2_K$. This can be seen via the increasing irregularities of the isolines.

Even though each value of $\sigma^2_K$ used the same number of MC realisations, the isoline bordering P10 (darkest shade of green) and P90 (white) increase in irregularity as the $\sigma^2_K$ is increased. The cause lie in the fact that lower numbers of realisations give rise
to P=0 (totally black in colour) and P=1 (white) when $\sigma^2_K$ is increased. This effect is obvious as the probability plotting program does not attempt to “smooth” out the lines, but plots them exactly at the prescribed level.

### 4.1.4 Behaviour along the well lines

Besides from calculating the spread in the capd, it is useful to view the behaviour of the probability values for each grid cell along the perpendicular and parallel lines centred on the pumping well. This will give a qualitative description of the behaviour of the capd as we move from West to East and North to South. The well lines are graphically defined in Figure 4-5.

![Figure 4-5: Imaginary perpendicular (blue) and parallel (red) lines running across the pumping well defined by y=400 and x=250.](image)

Two imaginary lines that cross the well can be described by y=400 and x=250 using the Cartesian axis set up in chapter 3. The line y=400 (shown in blue) runs from West to East while the line x=250 (shown in red) runs from North to South. These imaginary lines will be referred to as the West-East well line and the North-South
well line respectively. Analysis of the capd along these well lines for different $\sigma^2_k$ values can give a good initial representation of the changing behaviour of the capture zone. To do this, the probability distribution data file in Modflow is exported and altered so that it can be read in Matlab (see chapter 3). A script (m-file) was written to analyse the file and create a new file containing the probability values only for the desired grid cells along the well lines.

Figure 4-6 show the probability of capture for different variance values along the West-East well line when steady state has been reached.

The curves in Figure 4-6 suggest that along the West-East well line, the capd resembles a normal distribution pattern. As the variance increases, the distribution along the West-East line begins to spread, i.e. less grid cells with values of $P=0$ and $P=1$ and more values in between. This suggests an increase in the area of uncertainty ($0<P<1$) with higher $\sigma^2_k$ values.

Figure 4-7 show the probability of capture along the North-South well line for different variance values.
Figure 4-7: Probability of capture along the North-South well line for different variance values

Figure 4-7 shows that along the North-South well line, the capd resembles a cumulative normal distribution pattern. It is reversed because of the implemented Cartesian coordinates, i.e. y grid cell 500 is down-gradient of the pumping well. When comparing the results from Figure 4-6 and Figure 4-7, it can be seen that as $\sigma^2_K$ increases, the distribution pattern depart from normality. This becomes more significant as the distance between the cell grid and the pumping well increases - further up-gradient or down gradient from the extraction well. The well is located at $x=250$ and $y=400$.

The area of uncertainty is shown to increase for higher $\sigma^2_K$ by qualitative analyses of both well lines. Figure 4-7 also shows that the probability of capture of a particle located at large distances directly up-gradient from the pumping well is smaller for higher $\sigma^2_K$. This is seen by the drop in the curves when the up-gradient distance increases.

4.1.5 Behaviour of the capd areas P10, P50 and P90

Analysing the capture zone areas with a probability of capture higher than 10 percent (i.e. 20 percent or higher), higher than 50 percent (60 percent or higher) and 90 percent (100 percent capture) will give a description of the behaviour of uncertainty
as for different $\sigma^2_K$ values. These areas, P10, P50 and P90 respectively, are calculated from the truncated data files from Modflow (see chapter 3). A graphical representation of P10 and P90 areas are shown in Figure 4-8 for $\sigma^2_K = 1$ and 5.

Figure 4-8: P10 capture zone areas for $\sigma^2_K = 1$ (top left) and 5 (bottom left). P90 capture zone areas for $\sigma^2_K = 1$ (top right) and 5 (bottom right).

P90 is represents the capture zone area with high levels of certainty while P10 represents the capture zone area with low certainty. Their change in area with different $\sigma^2_K$ can therefore show the change in the ratio between capture certainties and capture uncertainties. The behaviour of these areas for different $\sigma^2_K$ values are shown in Figure 4-9.
Figure 4-9: Results of calculating the P10, P50 and P90 capture zone areas with increasing variance.

The capture zone area in Figure 4-9 is normalised to the capture zone area with a homogeneous assumption using the same parameters ($Q=-0.02 \text{ m}^3/\text{s}$, $\mu_K=10^{-11}\text{ m/s}$, $\nabla h=0.01$) in Section 4.1.1. This is seen by the fact that when the $\sigma^2_K=0$, in other words homogeneous, P10, P50 and P90 all have a value of 1. In doing this, the behaviour of the probability areas can be described relative to the expected homogeneous capture zone using the same aquifer and well properties.

It can be seen from Figure 4-9 that P10 increases dramatically when $\sigma^2_K$ is increased from 0 to 3. It then stabilises and increases at a slower rate when $\sigma^2_K$ is increased beyond 3. P90 follow an opposing pattern to P10 and decreases at a relatively high rate as $\sigma^2_K$ is increased from 0 to 2. The decrease slows down and stabilises after the $\sigma^2_K$ is higher than 3 but continues to decrease at a slower rate. The opposing trend in P10 and P90 is often observed when the fundamental homogeneous capture zone does not change with the varied parameter. In this case, the homogeneous capture area is always the same as it has a constant $\sigma^2_K=0$. On the other hand, for simulations such as varying the well extraction rate ($Q$), the homogeneous capture zone is expected to
decrease with lower extraction rates due to their fundamental relationship (quantifiable by Equation 2-17 in chapter 2). In these simulations, the trend between P10 and P90 may not always be opposed as they may both decrease with smaller Q. The opposing trend observed here can be explained by the fact that if P10 represents uncertainty in the capture zone while P90 represents certainty (or low levels of uncertainty) in the capture zone, it would be expected that when uncertainty increases, the associated certainty in the capture zone will decrease.

P50 shows a relatively stable trend in comparison to P10 and P90. This means that as the $\sigma^2_K$ is increased, the size of the median isochrone remains relatively unchanged, especially for $\sigma^2_K<3$. If the median isochrone is used as the statistical measure of the capd’s location, then Figure 4-9 show that the location of the capture zone remains relatively unchanged as $\sigma^2_K$ is increased up to 3 but shrinks when $\sigma^2_K$ is larger than 3.

**4.1.6 Influence of variance on the spread**

The calculated areas of P90 and P10 can be used to calculate the 80 percent zone of uncertainty. The 80 percent zone areal spread around the median isochrone can then be calculated using Equation 3-7 from chapter 3. The 80 percent areal spread is shown in Figure 4-10 for different $\sigma^2_K$ values.

![Figure 4-10: 80 percent areal spread around the median isochrone for different $\sigma^2_K$ values.](image-url)
Using a steady state time frame \((t \to \infty)\), Figure 4-10 shows that the 80 percent spread increases as \(\sigma^2_K\) is increased. The areal spread increases significantly when \(\sigma^2_K\) is increased from 0 to 2. This is due to the increasing P10 area and decreasing P90 area. As \(\sigma^2_K\) increases to 3 and 4 it stabilises as the ratios between P10 and P90 do not change significantly. The large jump in the areal spread when the variance reaches 5 is due to the drop in the P90 area to a value close to zero. Figure 4-10 suggests that as \(\sigma^2_K\) is increased, the areal spread increases at a decreasing rate in the range \(0<\sigma^2_K<4\). When \(\sigma^2_K\) reaches a value larger than 4, the spread becomes large due to low areas with \(P_{\text{capture}}=1\).

### 4.1.7 Discussion

As the heterogeneity of hydraulic conductivity of an aquifer increases, the uncertainty within the capture zone increases. The increasing uncertainty in determining the shape of the capture zone is reflected by the higher levels of irregularity in the isolines via visual analysis of the capd plots.

Along the well lines, the capd is found to resemble a normal distribution (West-East well line) and a cumulative normal distribution (North to South). As \(\sigma^2_K\) is increased though, the capd distribution departs from normality – increasing areas of uncertainty \((0<P<1)\). In particle transport research, several authors have found that for uniform flow the particle trajectories’ probability density function is practically normal for sufficiently small \(\sigma^2_K\) values or for large time for any \(\sigma^2_K\) values (e.g. Dagan and Fiori 1997). Van Leeuwen (2000) points out that this analogy only holds where the mean flow is uniform, that is, where particles are not too close to the well. The normality can be explained by the central limit theorem (CLT) as follows. The total particle travel distance to the well can be viewed as the sum of ‘m’ travel distances \(\Delta x\) in the grid cells visited by a particle. As ‘m’ is very large, and the random variables \(\Delta x\) have common probability distributions and are uncorrelated beyond the correlation length, it follows from the CLT that the sum \(\sum^m \Delta x\) tends to normality (van Leeuwen 2000).

The results in this simulation suggests that the particle trajectories’ probability density function departs from normality when \(\sigma^2_K\) is larger than 1. This, of course, is based on
the base parameters and model discretisation used. Nevertheless, based on the results in steady state, it can be seen that the probability of capture depart from normality for higher $\sigma^2_k$ values no matter how much time has elapsed. The normality behaviour is also influenced by the cell distance from the pumping well.

The analysis of P10, P50 and P90 areas show an increase in uncertainty in determining the size of the capture zone with increasing $\sigma^2_k$. Uncertainty in the size of the capture zone increases dramatically in the range of $0<\sigma^2_k<2$, before stabilising to a slower increase rate. The 80 percent areal spread calculation also confirms this behavioural pattern. The only conflicting result is the large areal spread resulting from $\sigma^2_k=5$. This is due to the decrease in the area of certainty (P90) and not an increase in the area of uncertainty (P10). The relationship between $\sigma^2_k$ and the areal spread depart from the predictable behaviour shown in the range $0<\sigma^2_k<4$ when $\sigma^2_k$ is higher than 4. The studies carried out by van Leeuwen (2000) also suggest that spread predictability is much higher at low $\sigma^2_k$ values. In his study, van Leeuwen (2000) suggests that for $\sigma^2_k$ between 0.1 and 0.5 in a confined aquifer, the spread in the capd increases linearly and is predictable.

The work carried out in this thesis suggests that the behaviour of the spread is non-linear with increasing $\sigma^2_k$. This is most significant when $\sigma^2_k$ is higher than 2. The areal spread seems to follow a more linear trend at the lower $\sigma^2_k$ range ($0<\sigma^2_k<2$) but the rate of increase in the spread decreases as $\sigma^2_k$ is increased in the range of $0<\sigma^2_k<4$. Since the areal spread is normalised with the expected capture zone calculated from homogeneous assumptions, it can also be concluded that as $\sigma^2_k$ increases, the assumption of homogeneity has lower validity.

From the analysis of the results presented, the general behaviour of the capture zone is as follows:

- as $\sigma^2_k$ is increased the shape of the capture zone becomes more uncertain;
- its spatial predictability departs from a normal distribution as $\sigma^2_k$ is increased;
- the predictability of the size of the capture zone decreases with increasing $\sigma^2_k$ – this is most significant between $\sigma^2_k$ values of 0 and 2;
• at lower $\sigma^2_K$ values ($\sigma^2_K<2$), the spread may be linearly dependent to the variance but for a larger $\sigma^2_K$ range it increases at a decreasing rate ($0<\sigma^2_K<4$);
• when $\sigma^2_K$ is larger than a certain value, the spread becomes unpredictable;
• and the location of the capture zone, based on visual analysis and the statistical median isochrone (P50), remains relatively unchanged at a lower range of $\sigma^2_K$ (in this case $0<\sigma^2_K<3$), but shrinks when $\sigma^2_K$ is larger than a certain valuing (this case $\sigma^2_K=3$) due to higher associated levels of uncertainty.

4.2 Isotropic correlation length of hydraulic conductivity

The aim in this simulation is to quantify the effects the isotropic correlation length ($C_L$) has on the capd. The main focus is to determine a general relationship between increasing correlation lengths in hydraulic conductivity and the resulting uncertainty within the capture zone. The influence of $C_L$ on the size, shape and location of the resulting capture zone can then be quantified by analysing the results.

Different values for the correlation length in hydraulic conductivity (all in meters) were used in this simulation. The values ranged from five to 1000 ($C_L=5, 10, 20, 30, 40, 100, 200, 500, 1000$). 10 MC simulations were carried out for each $C_L$ value resulting in a total of 90 different heterogeneous fields (10 for each $C_L$ value), 90 deterministic solutions and 9 stochastic capds.

All other parameters were kept constant at their standard values, i.e. $\sigma^2_K=3$, $Q=-0.02m^3/s$, $\nabla h = 0.01$ and $\mu_K=10^{-11}m/s$.

4.2.1 Homogeneous, random hydraulic conductivity ($C_L \to \infty$)

When the correlation length approaches infinity, the problem is that of a homogeneous aquifer with random hydraulic conductivity. For a fully confined aquifer, the problem can be solved analytically and has been done in past studies (e.g. van Leeuwen 2000). The stochastic results from van Leeuwen (2000) are shown in Figure 4-11.
The homogeneous hydraulic conductivity values are natural \(-\log\) normally distributed with a set statistical mean and variance. The solution results in a smooth, predictable capd with the probability of capture dependent on the location of the grid cell relative to the well, \(\nabla h\), \(Q\), the geometric mean of hydraulic conductivity and \(\sigma^2_K\).

### 4.2.2 Heterogeneous fields with increasing correlation length

For each of the nine correlation length values (5-1000), ten heterogeneous fields were created. Figure 4-12 shows one particular field of the 10 used for stochastic analysis for some of the correlation lengths used (not all).
It can be seen in Figure 4-12 that as the correlation length increases, areas of similar hydraulic conductivity values become significantly larger on the field. For $C_L=5$, the field changes hydraulic conductivity values over a short distance in comparison to larger $C_L$ which show larger areas of similar hydraulic conductivity.

### 4.2.3 Heterogeneous, stochastic results

The results of combining 10 MC simulations into a probability distribution for each of the 9 different correlation lengths are shown in Figure 4-13.

![Figure 4-13: Capds for different correlation lengths. From left to right, the correlation lengths for the top row are 5, 10, 20; middle row are 30, 40, 100; bottom row are 200, 500, 1000.](image)
Through visual analysis of the capd plots, as $C_L$ is increased from 5 to 100, the zone of uncertainty expands. The area of uncertainty then slowly stabilises and decreases as $C_L$ becomes higher than 100. This would suggest that there is an increase in uncertainty in determining the size of the capture zone as $C_L$ is increased from 5 to 100, but stabilises and decreases slightly for $C_L$ larger than 100.

Following from this observation, an interesting point is the fact that at low correlation lengths, the borders of the isolines are slightly more irregular in shape, even though the area of uncertainty is much smaller. The irregularity is due to the large spatial variability of hydraulic conductivity over a short distance for small $C_L$. Even though the area of uncertainty increases when the correlation length increases from 0 to 100, the irregularities of the borders smoothen out as the correlation length is increased from 0-1000. This suggests that as the $C_L$ increases from 0 to 100, even though the uncertainty in determining the size of the capture zone increases, the uncertainty in determining the shape may not.

### 4.2.4 Behaviour along the central lines

Figure 4-14 show the probability of capture for different $C_L$ values along the West-East well line when steady state has been reached (not all $C_L$ used are shown).
The curves in Figure 4-14 resemble a normal distribution pattern. As the isotropic correlation length increases from 5, the distribution along the West-East well line show an increase in the area of uncertainty (0<P<1). From Figure 4-14, the widest distribution with the largest area of uncertainty can be found for \( C_L =40 \) and \( C_L =100 \) (all lengths are in meters). As \( C_L \) increases beyond 100, the area of uncertainty begins to contract, as seen by the West-East well line distribution for \( C_L =1000 \). This suggests that more values of \( P=0 \) and \( P=1 \) can be found for correlation lengths that increase beyond \( C_L =100 \).

Figure 4-15 shows the probability of capture along the North-South well line for different correlation length values.

![Figure 4-15: Behaviour of the capd plot along the North-South well line for several (not all) correlation lengths.](image)

From Figure 4-15, the capd resembles a cumulative normal distribution pattern. It can be seen that the probability distribution pattern along the North-South well line departs from normality for certain correlation lengths – most notably the \( C_L =20, 40 \) and 100. Of these three correlation lengths, \( C_L =20 \) shows the closest behaviour to normality. From Figure 4-15, the behaviour along this well line is closest to normality when \( C_L =5 \) and \( C_L =1000 \).
When comparing the results of both Figure 4-15 and Figure 4-14, it can be seen that as the $C_L$ is increased from 5 to 100, the behaviour of the probability distribution pattern depart from normality. The probability of capture of a particle located directly up-gradient of the well at a large distance in this range also decrease for increasing $\nabla h$. The area of uncertainty also widens. These behaviours become more significant when the distance of the cell grid from the well increases. When $C_L$ increases past 100, the behaviour reverses and the probability of capture along both the West-East and North-South well line return to a normality pattern with a narrower spread. The results suggest that $C_L$ is increased up to a certain point, the probability distribution becomes less predictable. When the $C_L$ is increased past this point though, the behavioural pattern will reverse and the predictability in the capture zone will increase.

4.2.5 Behaviour of the capd areas P10, P50 and P90

Since the behavioural pattern of the probability distribution changes when $C_L$ is increased past a certain point, the results for the capd areas will be presented in two graphs. Figure 4-16 show the first of these graphs for the capd areas of P10, P50 and P90 for $C_L$ smaller than 100. Figure 4-17 then shows the data for a range of $C_L$ up to 1000.

![Capture zone area vs isotropic (in x-y) correlation lengths](image)

**Figure 4-16: Area of P10, P50 and P90 for correlation lengths of 5 to 100.**
Capture zone area vs isotropic (in x-y) correlation lengths

The change in P10 and P90 areas with increasing $C_L$ can show the behaviour of the ratio between the areas of certainty and uncertainty of capture. It can be seen from Figure 4-16 that P10 increases dramatically when $C_L$ is increased from 5 to 30. It then stabilises when $C_L$ is increased beyond 40. When the $C_L$ increases beyond 100, Figure 4-17 shows that P10 begins to decrease. Both Figure 4-16 and Figure 4-17 show that P90 follows an opposing pattern to P10 and decreases at a relatively high rate as the $C_L$ is initially increased from 5 to 40. In this range, the decreasing rate slows down and stabilises after $C_L=40$. As the $C_L$ increases beyond 100, the P90 area increases quite significantly. The opposing trend in P10 and P90 can again be explained by the fact that when all things (except one parameter) are kept equal, it would be expected that when uncertainty increases, the associated certainty in the capture zone will decrease.

With increasing correlation length, P50 shows a simular trend as P90 - except with higher levels of stability. P50 is shown to decrease when $C_L$ is increased from 5 to 40, but at a much slower rate than P90. As $C_L$ is increased beyond 40, it increases slightly up to $C_L=200$. Between $200<C_L<1000$, P50 remains relatively unchanged. If P50 is
used as the statistical measure of the capture zone’s location, then the he location of the capture zone will shrinks when $C_L$ increases from 5 to 40. This is due to the decrease in certainty (P90) and the increase in uncertainty (P10). When $C_L$ is increased beyond 40, the location expands in size up until $C_L = 200$ due to the increasing levels of certainty. When $C_L$ is larger than 200, the location of the capture zone becomes stable and remain relatively unchanged.

### 4.2.6 Influence of correlation length on the spread

The 80 percent zone areal spread around the median isochrone is shown in Figure 4-18 for different correlation lengths.

![80 percent areal spread for different correlation lengths](chart)

**Figure 4-18: 80 percent areal spread for different correlation lengths**

In steady state, the 80 percent spread increases when the correlation length is increased from 5 to 100. This is due to the increasing P10 (uncertainty) area and the decreasing P90 (certainty) area. It then starts to decrease when $C_L$ is larger than 100 due to a shrinking P10 and expanding P90 area.

An important observation about the influence of $C_L$ on the areal spread of the capture zone can be made in Figure 4-18. The behaviour of the spread with increasing $C_L$ resembles a natural-log normal distribution function shown in Figure 3-2 in chapter 3.
This is significant because it implies that the capture zone areal spread can be predicted from the correlation length for a given set of parameters (i.e. given variance, hydraulic gradient, pumping rate and mean hydraulic conductivity) in a confined aquifer at steady state.

### 4.2.7 Discussion

As the correlation structure of hydraulic conductivity of an aquifer increases up to a certain length, the uncertainty within the capture zone increases. Past a certain correlation length scale, the behaviour of uncertainty begins to stabilise and decrease. This correlation length is found to be at approximately $C_L=100$ for this simulation. The actual point at which uncertainty begins to stabilise and reverse in its behaviour will most likely depend on the base parameters used – such as the variance and mean of hydraulic conductivity, the background gradient and the well pumping rate. Nevertheless, from this set of simulations, the general behaviour of uncertainty with increasing correlation length can be described.

The increasing uncertainty in the shape of the capture zone is reflected by the increasing unevenness of the isolines bordering the isochrones. This irregularity is highest at small correlation lengths and can be seen via visual analysis of the stochastic capd plots. The irregularities at smaller correlation lengths is explained by the fact that the soil hydraulic conductivity changes significantly over relatively small distances in comparison to larger correlation lengths.

Along the well lines, the capture zone’s probability distribution departs from normality as $C_L$ is increased up to a certain point (~100). In this range, the predictability of the spatial probability variation decreases with larger correlation lengths. This result is especially visible for grid cells that are located further away from the well. After a certain correlation length (in these simulations, $C_L$ of 100), the behaviour of the capture probability falls back to normality. This can be explained by the fact that as $C_L$ increases and approaches infinity, the problem approaches that of a homogeneous aquifer with random hydraulic conductivity – i.e. the problem becomes more predictable as its solution becomes closer to the analytical solution used to predict the capd for a homogeneous aquifer with random hydraulic conductivity.
The behaviour of the probability of capture with increasing $C_L$ can be attributed to two conflicting, inter-correlated factors: the balance between the level of uncertainty driven by increasing $C_L$; and the level of certainty driven by the problem approaching a correlation length of infinity with a predictable, analytical solution. These two factors drive the level of normality of the behaviour along the well lines. At low correlation lengths, $C_L$ is much smaller than infinity, so the change in behaviour (increase) in uncertainty is due mostly to the change in the correlation structure. The rate of increase in uncertainty slows down as $C_L$ is increased. This is because the probabilities become more predictable as it approaches the analytical solution, resulting in higher levels of certainty and behaviour closer to the normal distribution. The point when these two factors balance out is around $C_L=100$ for this simulation.

The location of the capture zone, represented by P50, shrinks and expands as the $C_L$ is increased. Its behaviour follows the behaviour of the area of certainty (P90) but of less magnitude. This indicates that the location of the capture zone shrinks when the $C_L$ is increased up to a certain point ($C_L=100$ for this simulation). After this, when the $C_L$ is increased further, the location begins to expand due to higher levels of certainty. It then stabilises after a higher $C_L$ value ($C_L=200$ for this simulation) and remains relatively unchanged for subsequent increases in correlation length.

From analysis of the P10 and P90 areas, there is increasing uncertainty in determining the size of the capture zone as $C_L$ is increased from 5 to 100. When $C_L>100$, uncertainty decreases due to an increasing P90 area and a decreasing P10 area. The 80 percent areal spread calculation also confirms this behavioural pattern. Analysis of the areal spread suggests that it behaves similar to a natural-log normal function with different values of $C_L$. This is important because it means that the areal spread of a capture zone can be predicted given the correlation length. The shape of the natural-log normal function representing the relationship between the areal spread and $C_L$ is most likely dependent on other parameters such as the variance and mean of hydraulic conductivity, the well pumping rate and the background hydraulic gradient.

In the confined aquifer capture zone study carried out by van Leeuwen (2000) and the solute transport modelling study carried out by Dagan (1988), it was concluded that
the behaviour (and spread) of the probability of capture of a particle is insensitive to changes in the correlation structure. However, in his studies, van Leeuwen (2000) used a variance value of 0.5 and suggested that for large variance values, there should be dependence on the correlation structure. His reasoning behind this was because if the spread did not depend on the correlation structure, a large approximation of \( C_L \) (as \( C_L \rightarrow \infty \), the probability structure becomes more predictable) would always work. He also emphasised that for larger elapsed times (closer to steady state), the impact of the correlation structure should be felt at any variance value. He did not investigate these hypotheses though.

From the work carried out in this thesis, the areal spread in the probability of capture of a particle is dependent on the correlation structure, given a variance of 3 (base variance). This result does not conflict with the results in van Leeuwen’s study (2000) as the \( \sigma^2_K \) used is much larger. The results, however, confirms his hypothesis that at larger \( \sigma^2_K \) values, the spread is dependent on the correlation structure. This steady state simulation also confirms van Leeuwen’s prediction that for larger elapsed times, the influence of the correlation structure should be felt. The areal spread of the probability of capture was found to be natural-log normally dependent on \( C_L \). The fact that the spread is less sensitive to the correlation structure for small \( \sigma^2_K \) values may be explained by the prediction that the shape of the natural-log normal relationship is dependent on \( \sigma^2_K \). For instance, small \( \sigma^2_K \) values may distort the natural-log normal relationship between \( C_L \) and the areal spread to become much flatter – therefore changing the \( C_L \) in a certain range would hardly change the areal spread. It must be kept in mind that the curve should also be dependent on other factors such as \( \mu_K \), \( Q \) and \( \nabla h \).

From the analysis of the results presented, the general behaviour of the capture zone is as follows:

- as \( C_L \) is increased the shape of the capture zone becomes more certain due to decreasing irregularities bordering the isochrones;
- the spatial predictability of the capd departs from a normal distribution as the \( C_L \) is increased up to a point, then slowly falls back to normality;
the certainty in the size of the capture zone decreases with increasing $C_L$ until a certain point (100). The size becomes more predictable after this point;

- the areal spread of the probability of capture follows a natural-log normal relationship with $C_L$;

- and the location of the capture zone, based on visual analysis and the statistical median isochrone, shrinks as $C_L$ increases up to a certain point, after which it expands. Its behaviour corresponds to the level of certainty. Larger than a certain $C_L$ (200 in this simulation), the location of the capture zone remains unchanged.

### 4.3 Implementing anisotropic hydraulic conductivity

The aim in this simulation is to quantify the effects that anisotropic conditions have on the capd. The main focus is to determine a general relationship between levels of anisotropic conditions in hydraulic conductivity and the resulting uncertainty within the capture zone. The influence of anisotropy on the size, shape and location of the resulting capture zone can then be quantified by analysing the results.

Different levels of anisotropic conditions were used for these simulations. The ratio of correlation lengths in the x and y direction (i.e. $C_{LX}:C_{LY}$) were 1:5, 1:2, 1:1, 2:1 and 5:1. This experiment was done in two phases where the correlation length in the x direction ($C_{LX}$) was kept at 30 while the correlation length in the y direction ($C_{LY}$) was increased to 60 and 150. $C_{LY}$ would then be kept constant at 30 while $C_{LX}$ increased to 60 and 150. The results derived from the two phases were then combined to review the effects of anisotropy. In total, 10 heterogeneous fields were created for each anisotropic ratio, giving a total of 50 simulations. These were combined into 5 stochastic capds.

All other parameters were kept constant at their standard values, i.e. $\sigma^2_K = 3$, $Q = -0.02 m^3/s$, $\nabla h = 0.01$ and $\mu_K = 10^{-11} m/s$. 
4.3.1 Heterogeneous fields for varying anisotropic conditions

For each of the five different levels of anisotropy, ten heterogeneous fields were created. Figure 4-19 shows examples of one particular field of the 10 used for stochastic analyses for the five different levels of anisotropy.

![Figure 4-19: Heterogeneous fields created with different levels of anisotropy. From left to right, the top row have $C_{LX}:C_{LY}$ ratios of 1:5, 1:2 and 1:1. The second row have $C_{LX}:C_{LY}$ ratios 2:1 and 5:1.](image)

It can be seen in Figure 4-19 that as $C_L$ increases in one direction relative to the other, areas of similar hydraulic conductivity values become larger on the field in that direction. Areas of similar correlated hydraulic conductivity can be called lenses. Higher $C_{LY}$ result in ‘lenses’ in the soil being stretched in the y direction, and higher $C_{LX}$ results in lenses stretched in the x direction. Solving the individual field results in a heterogeneous, deterministic solution.
4.3.2 Heterogeneous, stochastic results

The results of combining 10 MC simulations into a probability distribution are shown in Figure 4-20.

Visual analysis of the capd plots suggest that uncertainties in the boundaries of the capture zone increase as the ratio of $C_{LX}:C_{LY}$ increase – that is, as $C_{LX}$ increases relative to $C_{LY}$. This behaviour is obvious judging from the higher levels of irregularity in the isolines, meaning a lower certainty in determining the shape of the capture zone. When $C_{LY}$ is large, the capture zone thins out and stretches in the y direction. When $C_{LX}$ is large, the capture zone begins to widen and stretch out in the x direction.
The area of uncertainty (0<P<1) increases with increasing $C_{LX}$. The area of certainty though, represented in white, also increases. The area of both certainty and uncertainty widens in the x direction with increasing $C_{LX}$. This can be explained by the fact that when $C_{LX}$ is increased, areas of similar hydraulic conductivity stretch in the x direction. This causes the probability of capture of a particle released in a particular grid cell to become more correlated to further grid cells in the x direction. This will hence enlarge the areas of similar capture probability in the x direction.

### 4.3.3 Behaviour along central lines

Figure 4-21 show the probability of capture for different levels of anisotropy along the West-East well line when steady state has been reached.

The curves in Figure 4-21 show that the probability distribution along the West-East well line begins to widen for increasing $C_{LX}$ values. The wider distribution suggests that there are more grid cells with probability values 0<P<1 as $C_{LX}$ increases. As $C_{LX}$ increases, the shape of the distribution also changes from a sharp, narrow normal distribution pattern into a wider, more parabolic relationship. This means that not only is the area of uncertainty becoming larger, the area of P=1 is becoming larger also.
while $P=0$ is decreasing. The change in the shape of the distribution may not necessarily mean a higher level of uncertainty, but simply a different pattern of relationship between the $x$ cell grid number and the probability of capture. From Figure 4-21, this changing relationship can be qualitatively described. Even though the area with $P=1$ is increasing, the higher number of uncertain grid cells ($0<P<1$) due to a smaller area of $P=0$ confirms that the area of uncertainty increases for higher $C_{LX}$.

Figure 4-22 shows the probability of capture along the North-South well line for different $C_{LX}:C_{LY}$ ratios.

![Behaviour of the capd from North to South (y axis at x=250)](image)

**Figure 4-22:** Behaviour of the capd along the North-South well lines for different levels of anisotropy.

From Figure 4-22, the graphs show that the behaviour of the capd departs from the cumulative normal distribution pattern along the North-South line for any level of anisotropy. The results indicate that along this well line, any level of anisotropy changes the capd distribution pattern, without differentiating whether it is an increase in $C_{LX}$ or $C_{LY}$. However, higher values of $C_{LX}$ creates a wider, more parabolic distribution while higher values of $C_{LY}$ still follow the cumulative normal pattern down-gradient of the well but departs from this behaviour further up-gradient. This means that for higher values of $C_{LX}$, the behaviour of the capd depart from normality when the distance from the well increases both down-gradient and up-gradient. For
higher values of \( C_{LY} \), the behaviour only departs from normality as the up-gradient distance increases.

### 4.3.4 Behaviour of the capd areas P10, P50 and P90

Since this simulation was carried out in two phases, Figure 4-23 shows the results from the two phases of simulation separately.

Examine Figure 4-23 separately is useful in determining the fact that when \( C_{LY} \) is increased while keeping \( C_{LX} \) constant, the areas of P10, P50 and P90 all decrease. When \( C_{LX} \) is increased while keeping \( C_{LY} \) constant, the areas of P10, P50 and P90 all increase. The behaviour of P10, P50 and P90 all follow the same pattern of increase or decrease. When the separate graphs are combined to reflect the level of anisotropy, the resulting graph is shown in Figure 4-24.
Figure 4-24: Combined graph of the two phases of simulations to show the relationship between the P10, P50 and P90 areas and different ratios of anisotropy.

The area of uncertainty (P10) and the area of certainty (P90) both increase with increasing ratio of $C_{LX}:C_{LY}$. At smaller ratio values, the rate of increase for both P10 and P90 areas is rapid. The rate of increase then slows down with increasing $C_{LX}:C_{LY}$. The magnitude of increase in P10, however, is much larger. This larger magnitude in P10 will mean that the area of uncertainty is increasing on a larger scale compared to the area of certainty.

The decreasing rate of increase in all the probability areas suggests that the areas of P10, P50 and P90 follow a polynomial relationship with the ratio of anisotropy. All areas display a pattern of variation similar to the polynomial relationship defined by:

$$f(x) = C\sqrt{x}$$

Equation 4-1

where $f(x)$ can represent the size of a capture zone with a predetermined probability (such as P10 or P90), $C$ is the coefficient of the polynomial and $x$ is the ratio of $C_{LX}:C_{LY}$ represented by $C_{LX}/C_{LY}$. The coefficient, $C$, in the equation determines the magnitude of the increase with increasing anisotropic ratio. Therefore the $C$ value used to predict the behaviour of the P90 area would be smaller than the $C$ value used to predict the P10 area. Since the ratio of $C_{LX}:C_{LY}$ used in these simulations ranged
from 0.2 to 2, this relationship is only plausible for \( C_{LX}:C_{LY} \) ratios within this range. The relationship for ratios outside this range needs to be proven via further simulations.

### 4.3.5 Influence of anisotropic conditions on the spread

The 80 percent areal spread around the median isochrone is shown in Figure 4-25 for different ratios of anisotropy.

![Figure 4-25: 80 percent areal spread for different levels of anisotropy.](image)

For anisotropic ratios between 0.2 and 5, if the polynomial relationship described by Equation 4-1 can be used to predict the P10 and P90 areas, then the resulting spread should, in theory, be linearly related in this range. Combining Equation 3-7 in chapter 3 to measure the 80 percent spread and Equation 4-1, the spread can be predicted using the relationship:

\[
f(x) = \left[ \frac{1}{4} \left( P_{10} - P_{90} \right) \right]^2 = \left[ \frac{1}{4} \left( C_{p10} \sqrt{x} - C_{p90} \sqrt{x} \right) \right]^2 = \frac{(C_{p10} - C_{p90})^2}{16} \cdot x
\]

**Equation 4-2**

where \( f(x) \) can represent the behaviour of the areal spread, \( C_{10} \) and \( C_{90} \) is the coefficients used for predicting the P10 and P90 area and \( x \) is the anisotropic ratio. From this derivation, the resulting relationship should be linear. Figure 4-25 shows
the experimental results display a strong linear relationship between the areal spread and the ratio of anisotropy for the first four points. The last point, at \( C_{LY}:C_{LY}=5 \), is slightly lower than expected from the predicted linear relationship. This can be explained by the interference of the domain size in the simulations. At \( C_{LY}:C_{LY}=5 \), the area of P10 is almost approaching 250000 square meters, which is the size of the domain. The theoretical P10 value for this level of anisotropy should actually be higher than the experimental P10 value recorded, as the experimental value is most likely limited by the size of the domain. This can also be seen via visual inspection of the capd in Figure 4-13, which shows the distortion of the capd along the borders of the model domain. The lower experimental value for P10 therefore contributes to the slightly lower experimental spread value compared to the predicted spread value using a linear relationship.

### 4.3.6 Discussion

As the level of anisotropy of hydraulic conductivity of an aquifer increases, the level of uncertainty in determining the capture zone changes depending on the direction of increasing anisotropy. If the level of anisotropy increases in the direction parallel to the background gradient \( (C_{LY}) \), the level of uncertainty decreases, while an increase in the level of anisotropy in the direction perpendicular to the background hydraulic gradient \( (C_{LY}) \) will increase this level of uncertainty.

Following from this analogy, visual inspection of the capds showed that the irregularity in the isolines increase as the \( C_{LY} \) is increased. This implies that the shape of a capture zone becomes less predictable when the correlation scale increases perpendicularly to the background hydraulic gradient.

Along the well lines, the capture zone’s probability distribution departs from normality for any level of anisotropy, regardless of direction. In both the well lines, higher \( C_{LY} \) causes the probability distribution to spread and tend toward a parabolic relationship, while high \( C_{LY} \) creates a narrower distribution. Using the North-South well line, the behaviour of the capd with larger \( C_{LY} \) values depart from the cumulative normal distribution both up-gradient and down-gradient of the pumping well. For large \( C_{LY} \) values, the behaviour only departs from normality up-gradient of the
pumping well. This behaviour is more significant when the distance from the well is increased. The change in behaviour of the capd with increasing levels of anisotropy along the well line can be visualised and their patterns of change quantified. The distribution along these well lines show that the zone of uncertainty (0<P<1) increases with higher $C_{LX}$ direction via the wider distributions.

Analysing the capd plots and the P10, P50 and P90 areas, it can be seen that all capture zone probability areas increase in size with higher levels of anisotropy in the x direction, regardless of the particular probability chosen. From the capd plots, the increase in area is visible in the direction of the anisotropic increase. This can be explained by the fact that increasing the correlation length in one direction creates larger areas of similar hydraulic conductivity in that direction and results in higher correlations in the probability of capture in that direction.

From analysis of the P10, P50 and P90 areas, the areas of uncertainty and certainty increase as $C_{LX}$ increases. The pattern of increase can be described by the square root polynomial function within the experimental range ($0.5 < C_{LX}:C_{LY} < 5$) of the level of anisotropy. The coefficients in the function are higher for levels of uncertainty (i.e. P10) compared to levels of certainty (i.e. P90).

The location of the capture zone, represented by P50, follows a similar behaviour described by the square root polynomial function. This indicates the location of the capture zone expands with increasing $C_{LX}$. The rate of expansion can be quantified by taking the derivative of Equation 4-1 and is shown in Equation 4-3:

$$f'(x) = Cx^{-\frac{3}{2}}$$

Equation 4-3

where $f'(x)$ represents the rate of expansion of the median isochrone, $C$ is a constant and $x$ represents the ratio of anisotropy. Equation 4-3 shows that the rate of expansion decreases with increasing ratio of anisotropy.

The 80 percent areal spread calculation also confirms the predicted behavioural pattern of P10, P50 and P90. Analysis of the areal spread suggests that it behaves
linearly with increasing anisotropy. This is important because it means that the areal spread of a capture zone can be predicted given the level of anisotropy. The magnitude (i.e. gradient) of the linearity relationship between the areal spread and the anisotropic level is most likely dependent on other parameters such as the $\sigma^2_K$ and $\mu_K$, $Q$ and $\nabla h$.

From the analysis of the results presented, the general behaviour of the capture zone for a confined aquifer at steady state is as follows:

- as the correlation length is increased in the direction perpendicular to the hydraulic gradient, the shape of the capture zone becomes less certain;
- the spatial predictability of the capd departs from a normal distribution for any level of anisotropy, but increasing the correlation length perpendicular to the hydraulic gradient creates a higher area of uncertainty;
- both the size of areas with high certainty and high uncertainty of capture increase with increasing correlation length perpendicular to the hydraulic gradient. Their behaviour follow a square root polynomial relationship with the ratio of anisotropy;
- the areal spread of the probability of capture follows a linear relationship with the ratio of anisotropy;
- and the location of the capture zone, based on visual analysis and the statistical median isochrone, expands when the correlation length is increased perpendicular to the hydraulic gradient. The rate of expansion can be quantified via the derivative of the square root polynomial equation.

An important point to note is the relationships between uncertainty and the shape, size and location of the capture zone for different ratios of anisotropy are derived in the range of $C_{LX}/C_{LY}$ of 0.2 to 5. Relationships beyond this range need to be proven via further experiments.

### 4.4 Background hydraulic gradient

The aim in this set of simulation is to quantify the effects of changing the background hydraulic gradient ($\nabla h$) on the capd. The main focus is to determine a general
relationship between $\nabla h$ and the resulting uncertainty within the capture zone. The influence of $\nabla h$ on the size, shape and location of the resulting capture zone can then be quantified by analysing the results.

Even though analytical solutions exist in determining the effects of $\nabla h$ on the capture zone area, they are formulated under the assumption of homogeneity. The simulations carried out in this section determine the size, shape and location of the capture zone in terms of probabilistic certainties under heterogeneous conditions. Besides from a qualitative and quantitative description of the absolute capd, the results in this section will be normalised against solutions derived from homogeneous assumptions. This normalisation technique can reflect the level of uncertainty in terms of the homogeneous capture zone – i.e. as a quantifiable deviation from the expected homogeneous capture zone.

The simulations used a hydraulic gradient of $\nabla h = 0.001, 0.009, 0.01, 0.02, 0.03, 0.05$ and $0.1$. Since the model had a constant head setting of $100m$ along the Southern boundary, the $\nabla h$ values are equivalent to allocating a constant head value of $99.5m$, $95.5m$, $95m$, $90m$, $85m$, $75m$ and $50m$ along the Northern boundary respectively. Note the domain size is $500m$ by $500m$. In total, $10$ heterogeneous fields were created for each $\nabla h$ value. This resulted in a total of $70$ separate simulations which was then combined into $7$ stochastic capds.

All other parameters were kept constant at their standard values, i.e. $\sigma_K^2 = 3$, $C_L = 20m$, $Q = -0.02m^3/s$ and $\mu_K = 10^{-11}m/s$.

### 4.4.1 Homogeneous, deterministic simulation

When the field has homogeneous hydraulic conductivity, the background hydraulic gradient can be related to the capture zone via the analytical solutions shown in Equation 2-17 to Equation 2-19 in chapter 2. From Equation 2-17, it can be seen that the capture zone is inversely proportional to the size of the capture zone – that is an increase in $\nabla h$ will result in a smaller capture zone. Several simulations were carried out under a homogeneous assumption for this domain and the results are shown in Figure 4-26.
When the capture zone areas were plotted against the hydraulic gradient, the results are shown in Figure 4-27.

From the graph, the values show that when $\nabla h$ is smaller than 0.02, the homogeneous capture zone area becomes extremely large. For this reason the data point for the $\nabla h=0.001$ was not included. When $\nabla h$ is initially increased, the capture zone area decreases rapidly. The rate of decrease slows down with further increases in $\nabla h$. It is important to note here that the area of importance lie in the range of $0.01<\nabla h < 0.1$, where the decrease in the capture zone is rapid but the absolute area is still small enough to be quantified by the modelling domain.
4.4.2 Heterogeneous, stochastic results

The generated heterogeneous maps had the same statistical values as the ones used in previous simulations ($\sigma^2_K = 3$, $C_L = 20 m$ and $\mu_K = 10^{-11} m/s$). The only variable that changed in this case was $\nabla h$, which was the constant head set at the Northern boundary in the modelling domain. When 10 MC realisations were combined for each hydraulic gradient value, the resulting capd plots are shown in Figure 4-28 (not all values are shown).

![Capd plots for different hydraulic gradients. From left to right, the top row has $\nabla h=0.001, 0.01$ and $0.02$, the bottom row has $\nabla h = 0.03, 0.05$ and 0.1.](image)

Qualitative analysis of the capd plots show that the uncertainties in the isolines do not change significantly with changing $\nabla h$. The irregularities remain fairly insensitive and display a similar pattern for all values of $\nabla h$. This suggests that the uncertainty in delineating the shape of the capture zone is insensitive to varying $\nabla h$. The uncertainty in determining the shape is most likely influenced by $\sigma^2_K$ and $C_L$ of the field as seen in previous simulations.

The uncertainty in determining the size of the capture zone is also hard to determine from visual inspection. Since both the white area ($P=1$) and the darkest green area
(P=0.1) decrease in size with increasing $\nabla h$, it becomes difficult to tell whether the ratios between $P=1$ and $P=0.1$ are changing. However, it is possible to conclude that the absolute size of all probabilities of capture shrink for higher values of $\nabla h$. This is expected as it resembles the homogeneous simulations carried out in the previous section.

A point to note here is the capd plot for $\nabla h=0.001$ and the extremely large areas of capture for all probabilities at this $\nabla h$ value show that there is an interference with the domain size. The domain boundaries are not large enough to accurately analysis the capd for this $\nabla h$ value and therefore, this data point will not be used in further quantitative assessment work.

### 4.4.3 Behaviour along central lines

Figure 4-29 shows the behaviour of the probabilities of capture along the West-East well line. Only 5 different values of hydraulic gradients are shown.

Figure 4-29: Behaviour of the capd along the West-East well line for different hydraulic gradients.
The base curve in Figure 4-29 is shown in dark blue with $\nabla h=0.01$. This is the standard curve used in previous simulations with all the standard base parameters. Analysis of the West-East well line shows that the distributions in the capd become narrower as the $\nabla h$ is increased. The narrower distribution in this case suggests that there are less grid cells with probability values in between $P=1$ and $P=0$, meaning a decrease in the area of uncertainty for increasing $\nabla h$. However, the area represented by $P=1$ also decreases with higher $\nabla h$. Only grid cells with $P=0$ increase with higher $\nabla h$ values. This means that the capture zone is decreasing in absolute size and is confirmed via visual inspection of the capd plots in the previous section.

It is hard to tell from Figure 4-29 whether or not the capd becomes more or less uncertain with different values of $\nabla h$. This is because all $\nabla h$ values show a similar pattern of regularity.

Figure 4-30 shows the probability of capture along the North-South well line for different $\nabla h$ values.

![Figure 4-30: Behaviour of the capd along the North-South well line for different hydraulic gradients.](image-url)
The blue line in Figure 4-30 is the base line used with a $\sigma^2_K = 3$ and $C_L = 20$. The slight departure from the cumulative normal distribution of this line is explained by the fact that $\sigma^2_K = 3$, in comparison to the graph used for $\sigma^2_K = 1$ in the first set of simulations. Along the North-South well line, it can be clearly seen that the capd behaviour departs from normality for higher values of $\nabla h$. The departure from normality continues to increase as $\nabla h$ is increased. This behaviour is especially true for cells located up-gradient from the well and becomes more significant as the distance increases.

Judging from Figure 4-30, it would seem that the probability of capture for an up-gradient grid cell is directly related to $\nabla h$. This can be seen by the fact that when we move further up-gradient, the probability of capture stabilises to a certain value for different $\nabla h$ values. For $\nabla h = 0.01, 0.02, 0.03, 0.05$ and 0.1, these probabilities can be estimated to be approximately $P=0.9, 0.5, 0.45, 0.35$ and 0.2. This hypothetical relationship is plotted in Figure 4-31.

![Figure 4-31: Hypothetical relationship between $\nabla h$ and the stabilising probability of capture at the up-gradient end.](image)

The estimated stabilising probability of capture at a large distance directly up-gradient of the well with increasing $\nabla h$ display a similar relationship to that between the homogeneous capture zone area and $\nabla h$. What the results show is that if we let $t \to \infty$, the probability of capture of a particle located at a large distance directly up-gradient of the well stabilises at a predictable, quantifiable value. Given certain aquifer
parameters and assuming that everything else remains unchanged, this quantifiable probability of capture shares a direct, inversely proportional relationship with $\nabla h$.

### 4.4.4 Behaviour of the capd areas P10, P50 and P90

The capture zone areas for P10, P50 and P90 are show in Figure 4-32.

![Figure 4-32: P10, P50 and P90 capture areas with different hydraulic gradients](image)

The areas of P10, P50 and P90 all show a similar trend to the homogeneous capture zone area with increasing $\nabla h$. This is expected because higher hydraulic gradients result in smaller capture zones, whether or not the simulations are carried in heterogeneous or homogeneous fields. Thus at smaller $\nabla h$ values, the areas of P10, P50 and P90 are large.

The result in Figure 4-32 is the absolute behaviour of the capds and can be attributed to two different factors. The first factor is the obvious one that higher $\nabla h$ values result in lower capture zone areas. They are fundamentally related in an inversely proportional manner and no matter how heterogeneous a field is, this factor will always influence each isochrone’s area. The second factor is that increasing $\nabla h$ may actually increase or decrease uncertainty within the capture zone. If this is so, another force will be driving the behaviour of the capd curves and at the same time changing the ratio between P10 (uncertainty) and P90 (certainty). Determining the second
factor is the aim for this simulation and the behaviour of the capd along the North-South line already indicate that uncertainty is influenced by $\nabla h$. To isolate the second factor, Figure 4-32 can be normalised to the equivalent homogeneous capture zone areas (based on the same parameters except $\sigma_k=C_l=0$) for each $\nabla h$ value. The calculated homogeneous capture zone area was carried out and explained in Section 4.4.1. This will take away the effects of the first factor and the results are shown in Figure 4-33.

![Figure 4-33: P10, P50 and P90 capture areas with different hydraulic gradients](image)

From Figure 4-33, it is now clear that $\nabla h$ does influence the uncertainty in a capture zone. The ratio of between P10 and P90 show an obvious decrease in areas of certainty in proportion to the areas of uncertainty. On a scale of relativity, the capture zone becomes more uncertain when $\nabla h$ is increased. That is, uncertainty measured against the expected capture zone area (derived from homogeneity). Initial estimations were far from this result as both the absolute capd areas (Figure 4-32), the qualitative capd plots (Figure 4-28) and the homogeneous capture zone areas all showed a decreasing relationship between $\nabla h$ and the capture area. This result, however, confirms with the results derived from the North-South well line that $\nabla h$ increases uncertainty. The North-South well line simply showed a lower stabilising probability up-gradient of the pumping well with increasing $\nabla h$. 
In terms of P50, the results show that its deviation from the homogeneous capture zone remains relatively unchanged between $\nabla h$ values of 0.01 and 0.03. This indicates that the uncertainty in determining the location of the capture zone is less sensitive to $\nabla h$ in this range. When $\nabla h$ is larger than 0.03, the median isochrone begins to shrink relative to the expected homogeneous capture zone. This is due to the increasing uncertainty in determining the location of the capture zone. The rate of deviation, however, is fairly slow even for an increase of $\nabla h$ of more than three folds. Although the level of uncertainty in the location of the capture zone relative to the homogeneous capture zone is shown by the normalised P50 in Figure 4-33, in absolute terms (Figure 4-32), the location of the capture zone shrinks rapidly in the range of $0.001 < \nabla h < 0.05$.

### 4.4.5 Influence of hydraulic gradient on the capd spread

The 80 percent spread calculated from the P10 and P90 values are shown in Figure 4-34.

![Figure 4-34: 80 percent areal spread with different $\nabla h$ values. Note this is the absolute values.](image)

This graph measures the absolute areal spread and once again, its behaviour is attributed to two factors – the decreasing size of the capture zone with increasing $\nabla h$; and the change in ratio between P10 and P90 reflecting changes in the level of
uncertainty with increasing $\nabla h$. To see the behaviour of the areal spread driven by changes in the ratio of P10 and P90, the normalised results are shown in Figure 4-35.

![Figure 4-35: 80 percent areal spread of the capd normalised against the homogeneous area for different $\nabla h$ values.](image)

Figure 4-35 shows clearly that the areal spread, relative to the homogeneous capture zone size, increases with increasing $\nabla h$. This suggests that the spread in the smaller capture zone areas (absolute area), created by higher $\nabla h$, display more uncertainty.

Another interesting point from Figure 4-35 is that the increase in spread attributed to increasing $\nabla h$ follows a strong linear pattern for the tested range. This is a significant finding since we know that when $\nabla h$ increases, the capture zone area will shrink, but the quantifiable level of uncertainty will increase linearly. This is useful for applications such as risk assessment analyses, whereby the average measured $\nabla h$ can be used to estimate the capture zone area via a homogeneous assumption and then the linearly related level of associated uncertainty can be factored in.

### 4.4.6 Discussion

Qualitative analysis of the capd plots show that the uncertainties in the isolines do not change significantly with changing $\nabla h$, indicating insensitivity of $\nabla h$ to the level of
uncertainty in determining the shape of the capture zone. The size of the capture zone, however, decreases noticeably with increasing $\nabla h$. This is expected from the simulations carried out under homogeneous assumptions.

Analyses along the well lines show that the capd distribution from West to East behaves similar to a normal distribution and lower $\nabla h$ values result in wider distributions. Although there is a change in the width of the distribution, the patterns of the capd do not depart much from normality and show similar regularities. This means moving in the direction perpendicular to the hydraulic gradient, $\nabla h$ does not really change the capd’s predictability in this direction.

Along the North-South well line, the probabilities depart from the cumulative normal pattern as $\nabla h$ increases. With higher values of $\nabla h$, the up-gradient probability of capture decreases. The up-gradient probability of capture can be quantifiably related to $\nabla h$ as values stabilise at distinctively different levels for different $\nabla h$ values. The results show that the probability of capture for a particle located at any large distance up-gradient and in line with the pumping well is inversely proportional to the hydraulic gradient. This relationship is only quantifiable as $t\rightarrow\infty$. The results from this well line show that higher $\nabla h$ values are associated with lower probabilities of capture, especially as the distance from the well increases.

The behaviour of P10, P50 and P90 are driven by two factors, namely the decreasing capture area with increasing $\nabla h$ and the change between the ratio of areas of certainty and uncertainty with increasing $\nabla h$. The changes in the level of uncertainty was quantified via normalisation and found that higher levels of uncertainty are associated with higher $\nabla h$ values. This result confirms the results derived from the North-South line.

The location of the median isochrone, used to define the location of a capture zone, is smaller for higher $\nabla h$ values in terms of absolute size and follows a similar relationship as the expected homogeneous capture area. The normalised P50 area show that the location of the capture zone with different $\nabla h$ values do not deviate much from the expected homogeneous capture zone when $\nabla h <0.03$. This is due to
the higher levels of certainty associated with lower $\nabla h$ values. From $\nabla h = 0.03$ to 0.1, the location shrinks slightly in size compared to the expected homogeneous capture zone due to higher levels of uncertainty.

The behaviour of the absolute areal spread is also driven by the two aforementioned factors, and isolating uncertainty driven by $\nabla h$ relative to the homogeneous capture zone area confirmed that relatively higher spreads occur for smaller capture zones. This means that smaller capture zones produced by higher $\nabla h$ have higher levels of deviation from the expected homogeneous behaviour. Even though the absolute spread and probabilistic capture area decreases with higher $\nabla h$ values, higher $\nabla h$ values are associated with higher levels of risk and uncertainty. The deviation from the homogeneous capture zone is shown to increase linearly with increasing $\nabla h$. The magnitude of increase (gradient) should depend on other parameters such as the mean, variance and correlation length of hydraulic conductivity and the well extraction rate.

Based on the results from this simulation, the behaviour of the capture zone is as follows:

- The absolute size of the capture zone is expected, and is confirmed to decrease with higher values of $\nabla h$ based on their inversely proportional fundamental relationship, even in a heterogeneous setting;
- The level of uncertainty in determining the shape of the capture zone remain relatively unchanged with different values of $\nabla h$;
- Along the well line in the direction perpendicular to the hydraulic gradient, the capd follow a normal distribution pattern with higher spreads attributed to lower $\nabla h$ values;
- In the direction parallel to the hydraulic gradient, the probability of capture of a particle up-gradient and in line with the well for large distances is quantifiable via an inversely proportional relationship between $\nabla h$ and $P_{\text{capture}}$. This is only valid as $t \to \infty$;
- Higher levels of uncertainty are associated with smaller capture zones for higher $\nabla h$;
- The relative 80 percent spread, which shows the expected deviation from the homogeneous capture zone, increases linearly with $\nabla h$;
The deviation of P50 from the homogeneous capture zone area remains fairly constant for changes in $\nabla h$ in the range of $0.01 < \nabla h < 0.03$ due to higher levels of certainty. The location shrinks slightly (relative to the expected homogeneous capture zone) as $\nabla h$ increases from 0.03 to 0.1 due to higher levels of associated uncertainty at higher $\nabla h$ values.

4.5 Well pumping (extraction) rate

The aim in this simulation is to quantify the effects of changing the well extraction rate ($Q$) on the capd. The main focus is to determine a general relationship between the well extraction rate and the resulting uncertainty within the capture zone. The influence of the extraction rate on the size, shape and location of the resulting capture zone can then be quantified by analysing the results.

The influence of the well extraction rate on a capture zone is well studied and analytical solutions exist in determining how it affects the capture zone. These solutions, however, are formulated under the assumption of homogeneity. The simulations carried out in this section determine the influence of a pumping well’s extraction rate on the capture zone in terms of probabilistic certainties under heterogeneous conditions. Besides from a qualitative and quantitative description of the absolute capd, the results in this section will again be normalised against solutions derived from homogeneous assumptions. This normalisation technique can reflect the level deviation from the homogeneous capture zone.

This section deviates slightly from other sections as it also examines different pumping rates for different variances of hydraulic conductivity ($\sigma_k^2$). This changes two variables at once and is aimed to confirm whether or not the behaviour in uncertainty for different extraction rates, derived for one $\sigma_k^2$ value, holds for other $\sigma_k^2$ values.

The simulations used a base standard pumping rate of $Q = 0.02 \text{ m}^3/\text{s}$. It was varied to $Q = 0.01 \text{ m}^3/\text{s}$ and $Q = 0.004 \text{ m}^3/\text{s}$. These extraction rates are equivalent to one-half and one-fifth of the base extraction rate, i.e. $Q_b/2$ and $Q_b/5$. The 3 different pumping rates were varied under 3 different variance values of $\sigma_k^2 = 1, 3$ and 5. This resulted in a
total of 30 separate simulations for the different pumping rates using one variance value. Since there were 3 variance values, a total of 90 deterministic solutions were used for this section. This resulted in 9 stochastic capds, 3 for each variance value. All pumping rates, Q, will be in units m$^3$/s unless stated otherwise. The units will be omitted for convenience.

The well was still located at the Cartesian coordinates of x=250, y=400 and all other parameters besides $\sigma_K^2$ and the Q were kept constant at their standard values, i.e. correlation length=20m, $\nabla h=0.01$ and $\mu_K=10^{-11}$m/s.

4.5.1 Homogeneous, deterministic simulation

For a homogeneous hydraulic conductivity setting, the well extraction rate can be related to the capture zone via the analytical solutions shown in Equation 2-17 to Equation 2-19 in chapter 2. From Equation 2-17, it can be seen that the capture zone increases in size for higher extraction rates. Using the base parameters, three simulations using different Q were carried out under a homogeneous assumption. The results are shown in Figure 4-36.

Figure 4-36: Homogeneous capture zones for different pumping rates. From left to right, Q=0.02, 0.004 and 0.01.

When the capture zone area is plotted against the well extraction rate for the given domain and base parameters used, it results in a linear relationship. This is shown in Figure 4-37.
The size of the homogeneous capture zone for this domain can be easily predicted for different extraction rates from this linear relationship. The goal of the heterogeneous simulations is thus to quantify the deviation from this trend. This can be done via normalisation against the expected homogeneous behaviour.

### 4.5.2 Heterogeneous, stochastic results

Combining 90 solutions, the resulting 9 stochastic capds are shown in Figure 4-38 ($\sigma^2_{K}=1$), Figure 4-39 ($\sigma^2_{K}=3$) and Figure 4-40 ($\sigma^2_{K}=5$).
Analysis of the capd plots show that the uncertainties in the isolines do not change significantly with changing pumping rates. The level of irregularities remains fairly insensitive and displays a similar pattern for all values of Q. The irregularities are, however, driven by increasing $\sigma_k^2$. This suggests that the uncertainty in delineating the shape of the capture zone is insensitive to varying Q. Careful close examination may show that irregularities increase slightly for smaller Q values at large distances up-gradient. However, this cannot be confirmed without further analysis.

The level of uncertainty in determining the size of the capture zone is also hard to determine from visual inspection. Since both the white area (P=1) and the darkest green area (P=0.1) decrease in size with decreasing Q, it becomes difficult to tell whether the ratios between areas of P=1 and P=0.1 are changing. However, it is possible to conclude that the absolute size of all probabilities of capture shrink for
lower values of Q. This is expected as it resembles the homogeneous simulations carried out in the previous section.

4.5.3 Behaviour along central lines

Figure 4-41, Figure 4-42 and Figure 4-43 show the behaviour of the capd along the West-East well line for different pumping rates under a variance of 1, 3 and 5 respectively.

Figure 4-41: Behaviour of the capd along the West-East well line for different pumping rates and $\sigma_k^2=1$.

Figure 4-42: Behaviour of the capd along the West-East well line for different pumping rates and $\sigma_k^2=3$. 
Figure 4-43: Behaviour of the capd along the West-East well line for different pumping rates and \( \sigma_k^2 = 5 \).

It can be seen that moving from West to East along the well line, higher Q values widen the normal like distribution. This is expected as a higher Q gives a larger width in the capture area. What cannot be determined is the change in ratio between the area of uncertainty (0<P<1) and grid cells with P=1, since they both decrease as Q decreases. This is seen via the narrower distribution and sharper peak with lower Q values. Nevertheless, along this well line, the pumping rate does not distort the general pattern of normality but only widens the distribution at the bottom and top for larger Q values.

From the 3 separate graphs, it can be seen that the change in the behaviour of the capd is almost identical for all variance levels. That is, a larger Q will always widen the distribution in the same way. The only difference for varying levels \( \sigma_k^2 \) is that the probabilities become slightly more spread between grid cells 200 to 300 for larger \( \sigma_k^2 \). This is consistent for all levels of extraction, and is therefore due mainly to the changing \( \sigma_k^2 \). However, careful examinations of the results show that lower Q values are slightly more affected by the increasing \( \sigma_k^2 \). This suggests that for lower extraction rates, the level of uncertainty in the capture zone may be more affected by the heterogeneity in the soil.
Figure 4-44, Figure 4-45 and Figure 4-46 show the behaviour of the capd along the North-South well lines for different extraction rates for a variance of 1, 3 and 5 respectively.

Figure 4-44: Behaviour of the capd along the North-South well line for different pumping rates and a variance of 1.

Figure 4-45: Behaviour of the capd along the North-South well line for different pumping rates and a variance of 3.
Along the North-South well line, the pumping rate influences the pattern of behaviour of the capd. The general cumulative normal distribution trend is replaced by a curve with an oscillating pattern up-gradient of the well. As the distance from the well increases, the oscillation decreases in amplitude and stabilises to a certain value. This behaviour occurs irrespective of $\sigma^2_K$ and suggests that it is driven entirely by decreasing the pumping rate. The fact that this pattern is displayed for all $\sigma^2_K$ values and the stabilisation of the probability of capture as we move further up-gradient confirms that it is not due to the convergence of the MC realisations. The amplitude of the second peak is exactly the same size for all $\sigma^2_K$ and occurs at a similar location (around grid cell 200) for all $\sigma^2_K$. Increasing $\sigma^2_K$ simply shifts the oscillating curve in a downward direction, especially for larger distances up-gradient. This has been quantified and confirmed by the previous investigation.

The fluctuating behaviour of the capd along the North-South well-line means an increase in uncertainty in determining the probabilities of capture for smaller values of Q. It does not necessarily mean a larger area of uncertainty ($0<P<1$). For large distances up-gradient from the well, the probability of capture stabilises to a certain value. This value is determined by both Q and $\sigma^2_K$. A higher $\sigma^2_K$ and a lower Q will result in smaller probability of capture for large distances up-gradient.
4.5.4 Behaviour of the capd areas P10, P50 and P90

The capture zone areas of P10, P50 and P90 are shown in Figure 4-47, Figure 4-48 and Figure 4-49. The results are presented separately for each probability of capture along with the different $\sigma_K^2$ values.

Figure 4-47: P10 area for a variance of 1, 3 and 5 for different values of Q.

Figure 4-48: P50 area for a variance of 1, 3 and 5 for different values of Q.
The areas of P10, P50 and P90 all show a similar trend to the homogeneous capture zone area with increasing extraction rate. The strong linear trend in the increase can be attributed to the fundamental behaviour of a homogeneous capture zone expanding linearly with increasing Q. The increase in \( \sigma_K^2 \) seems to ‘spread’ the probabilistic areal curves and divert it from homogeneous linear behaviour. This suggests that the higher \( \sigma_K^2 \) enhance the behavioural trend of uncertainty associated with changing Q, and decreases the significance of the fundamental behaviour caused by homogeneity. This is especially true for P90.

The results are consistent with previous simulations and confirm that for higher \( \sigma_K^2 \), P10 will be higher and P90 will be lower, for any pumping rate. The P50 area is always larger for lower \( \sigma_K^2 \) for all pumping rates. This is because for lower \( \sigma_K^2 \), there is a higher certainty in delineating the location of the capture zone through the median isochrone.

The effects of changing the extraction rate, however, are hard to assess due to the strong linearity in the behaviour of the graphs. The changing behaviour of all P10, P50 and P90 areas with increasing Q for a given \( \sigma_K^2 \) can once again be attributed to two different factors. The first factor is the fundamental positive linear relationship between a capture zone size and the well extraction rate. The second factor is that changing the extraction rate may actually increase or decrease uncertainty within the capture zone. If this is so, the second factor may be changing the ratio between P10

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Figure 4-49: P90 area for a variance of 1, 3 and 5 for different values of Q.
(uncertainty) and P90 (certainty), but its effects are over-shadowed by the first factor. Determining the second factor is the aim for this set of simulations and the behaviour of the capd along the North-South line already indicate that uncertainty is influenced by both the $\sigma^2_K$ and Q. To isolate the second factor, the probabilistic capture zone areas will again be normalised to the equivalent homogeneous capture zone areas (based on the same parameters except $\sigma_K=C_L=0$) for each Q value. This will take away the effects of the first factor and the results are shown in Figure 4-50.

From Figure 4-50, it becomes obvious that uncertainty decreases for higher levels of Q. The decreasing normalised P10 area and increasing normalised P90 area shows that the capd will behave closer to the homogeneous capture zone for higher extraction rates. The results show that as $Q \to 0$, the absolute size of the capture zone will become very small (seen in Figure 4-47, Figure 4-48 and Figure 4-49). However,
the uncertainty associated with a small Q becomes infinitely large. This is shown in Figure 4-50 where P10→∞ and P90→0 (note this is when t→∞, or at steady state).

The different σ²K values plotted on the graph confirm that P10, P50 and P90 all follow a similar behaviour regardless of σ²K. The variance enhances this behaviour caused by different pumping rates. For all variances, as Q increases, P10 decreases at a decreasing rate and P50 and P90 increase at a decreasing rate.

The P50 area used to define the location of a capd can be seen to follow the behaviour of areas of high certainty (P90). When Q is increased in the range of 0.004 to 0.01, the location of the capd expands faster than the homogeneous capture area due to increases in the levels of certainty on top of the expected fundamental linear increase. The normalised result show that when Q is increased above 0.01, the deviation from homogeneity stabilises. This suggests that the location of the capture zone increases fairly linearly following the homogeneous capture zone behaviour. The stabilisation of the normalised P50 with increasing Q occurs at lower values of Q for lower σ²K, meaning the lower the variance, the lower the Q value needed for the capture zone to behave like the homogeneous capture zone.

### 4.5.5 Influence of variance on the spread

The normalised 80 percent areal spread for different pumping rates are shown in Figure 4-51 for σ²K=1, 3 and 5.
Figure 4-51: Normalised 80 percent spread for different pumping rates and variances.

Even though no extraction will result in a spread of 0, Figure 4-51 shows that as \( Q \to 0 \), the areal spread approaches infinity. This means that under heterogeneous conditions, decreasing the extraction rate will make the probabilistic capture zone behave further and further away from the expected homogeneous capture zone, i.e. higher and higher levels of uncertainty. This happens regardless of \( \sigma^2_K \).

However, the uncertainty decreases at a slower rate for larger extraction rates and stabilises to a certain value. This value is higher for larger \( \sigma^2_K \). This means that increasing \( Q \) will increase the certainty in the capture zone, but if \( Q \) was increased to an infinitely large value, there will still be a quantifiable level of uncertainty that would remain. This quantifiable level of uncertainty is where the graph stabilises and any subsequent increase in \( Q \) will hardly change the spread. \( \sigma^2_K \) influences this point and larger \( \sigma^2_K \) gives a higher level of uncertainty for an infinitely large \( Q \), i.e. as \( Q \to \infty \) and \( t \to \infty \), the areal spread approaches a value depending on \( \sigma^2_K \).
4.5.6 Discussion

Increasing Q is shown to increase the absolute area of capture, under both homogeneous and heterogeneous formations. This can be seen from the homogeneous capture zone areas and the capd plots, and is confirmed through further quantitative analyses of the homogeneous capture zone area and P10, P50 and P90.

Along the West-East well-line, higher Q values widen the normal like distribution due mainly to the larger width in the capture zone created by higher extraction rates. Along this well line, the pumping rate does not distort the general pattern of normality but only changes the width of the distribution, regardless of the variance. Careful examinations of the results also showed that lower Q values are slightly more affected by the increasing variance. This suggests that for lower extraction rates, the level of uncertainty in the capture zone may be more affected by the heterogeneity in the soil.

The behaviour of the capd along the North-South well line and up-gradient from the well can be quantified by the separate influences of the pumping rate and the variance. First we have to assume that for low heterogeneity and high pumping rates, the capd behaviour along the North-South well line roughly resembles that of a cumulative normal distribution. This has been proven in previous simulations. Secondly, the effect of increasing the variance can be seen in this simulation and previous simulations. Increasing the variance shifts the up-gradient tail of the capd downwards, and this behaviour increases in significance further away from the well. Thirdly, from the results of this simulation, lowering the extraction rate changes the behavioural pattern of the capd along the North-South well line. Up-gradient from the well, it implements a filtering type function onto the capd such as the function \( f'(x) = \text{sinc}(x) \). Sinc(x) is the product of the trigonometric function \( \sin(x) \) and a monotonically decreasing function, such as \( 1/x \). The significance of the filtering function behaviour of the capd along the North-South well-line is dependent on the ratio of between Q to \( \sigma^2_K \). That is for smaller values of Q and higher values of \( \sigma^2_K \), the higher the influence of the filtering function. The period of the function occurs at the same place for all variance levels and may be related to \( C_L \). Nevertheless, the fluctuating behaviour of the capd along the North-South well-line means an increase in uncertainty in determining the probabilities of capture for smaller values of Q.
The probability of capture of a particle located at a large distance directly up-gradient of the well stabilises to a certain value for all $\sigma^2_K$ and $Q$ values. This value is determined by both $Q$ and $\sigma^2_K$. The higher the variance and the lower the extraction rate, the smaller the probability of capture for large distances up-gradient.

The observations along the well lines can be explained by the following rationale. Particles released at a certain point have a potential of being captured by the extraction well. However, for lower extraction rates, the particles will spend more time in the porous medium before they are captured in comparison to a higher extraction rate (on average). The longer travel times for the average particle means they encounter more heterogeneity and results in a higher probability that they will be caught in areas of low hydraulic conductivity. Therefore, the probability of capture of particles directly up-gradient may be lower and display a higher level of fluctuation due to the longer travel times. This also explains the observation that lower extraction rates are more affected by the heterogeneity of the soil since the longer travel times results in a higher probability that a particle encounters areas of low hydraulic conductivity. The same behaviour is seen in solute dispersion where the ensemble longitudinal variance with respect to the expected plume centroid is found to increase with the travel time (e.g. Bellin et. al. 1992).

Even though the absolute capture area is shown to increase with higher $Q$, the uncertainties caused by different extraction rates can only be seen via normalisation of the results. The normalised P10, P50 and P90 areas showed that uncertainty becomes extremely large when $Q$ becomes infinitely small. The normalised areal spread, or deviation from the homogeneous capture zone, for different extraction rates can be quantitatively described to follow a reciprocal type function for $Q>0$ and $t\to\infty$. This is defined by:

$$f(x) = \frac{ax + b}{x} = a + \frac{b}{x}$$

*Equation 4-4*
where in this case the function $f(x)$ represents the normalised spread or deviation from the homogeneous assumption, $x$ is the pumping rate $Q$ and $a$ and $b$ are constants. The constant $b$ determines the sharpness of the curve, i.e. the rate of decrease and stabilisation. A higher $b$ values makes the curve less sharp, which means decreasing and stabilising at slower rates. The constant $b$ is most likely dependent on the other aquifer properties such as $C_L$, $\mu_K$ and $\nabla h$. The effects of these parameters on the curve can only be determined via further dual variable simulations with $Q$, such as the simulation carried out here with $Q$ and $\sigma^2_K$.

However, this simulation has determined that the constant ‘$a$’ is affected by the variance. The constant ‘$a$’ changes the value of the limit that the function approaches when $x$ (or $Q$ in this case) approaches infinity. Higher values of ‘$a$’ means a higher limit. The normalised spread in this simulation, for example, can be described by Equation 4-4 and a variance of 1, 3 and 5 corresponds to approximate ‘$a$’ values of $a \approx 0.1$, 0.3 and 0.6 respectively. The value of ‘$a$’ is representative of the minimum level of uncertainty (or deviation from the homogeneous capture zone) no matter how large $Q$ is.

Based on the results from this simulation, the behaviour of the capture zone is as follows:

- The absolute size of the capture zone is expected, and is confirmed to increase with higher values of $Q$ regardless of a homogeneous or heterogeneous formation;
- The level of uncertainty in determining the shape of the capture zone driven by changes in $Q$ is difficult to assess but increases $\sigma^2_K$ show higher levels of uncertainty through irregularities in the isolines;
- The normal capd behaviour along the West-East well line widens with higher $Q$ due to increases in the width of the capture zone. Along the North-South well line, low $Q$ and high $\sigma^2_K$ changes the cumulative normal pattern into a filtering function of decreasing amplitude reflecting higher uncertainty in determining the probability of capture;
- Along the well lines, lower extraction rates are more effected by heterogeneity;
• The probability of capture of a particle up-gradient and in line with the well for large distances is quantifiable (stabilises) and depends on both $\sigma_k^2$ and $Q$. Higher $Q$ and lower $\sigma_k^2$ means higher $P_{\text{capture}}$.

• The normalised spread, or deviation from a homogeneous assumption, is related to $Q$ via a reciprocal relationship with $\sigma_k^2$ determining a coefficient;

• The location of the capture zone expands in absolute size as $Q$ increases due to the fundamental analytical relationship. However, it expands at a faster rate than the homogeneous assumption due to increases in levels of certainty associated with higher $Q$.

4.6 Dual well simulation – Varying the well spacing parallel to the hydraulic gradient

Two extraction wells are used in this simulation. The aim is to quantify the effects of changing the parallel well spacing on the capd. The main focus is to determine a general relationship between the distance in well spacing in the direction parallel to the hydraulic gradient and the resulting uncertainty within the capture zone. The influence of parallel well spacing on the size, shape and location of the resulting capture zone can then be quantified by analysing the results.

Besides from a qualitative and quantitative description of the absolute capd, the results in this section will again be compared to the solutions derived from homogeneous assumptions. This will show the level of uncertainty via the amount of deviation from a homogeneous assumption.

The simulations used a parallel well spacing of 0, 4, 10, 20, 40 and 100 (all in meters). The well spacings corresponded to 0, 1/5, ½, 1, 2 and 5 times the heterogeneous correlation structure of the field. The extraction rate used was half the extraction rate of the single well simulations, i.e. 0.01m$^3$/s. This was chosen so a direct comparison can be seen via using the same total extraction rate (0.02m$^3$/s). One well was kept at the standard location (x=250, y=400), while the second well was gradually spaced in the $y$ direction (at x=250, y=396, 390, 380, 360 and 300).
In total, 10 heterogeneous fields were created for each of the well spacing values. This resulted in a total of 60 separate deterministic simulations being used for this section. The MC analysis produced 6 stochastic capds.

All other parameters were kept constant at their standard values except for the pumping rate of each well ($Q_b/2$) and the well spacing, i.e. $\sigma_k^2 = 3$, $C_L = 20$, $\nabla h = 0.01$, and $\mu_K = 10^{-11}$ m/s. The units for the spacings (in meters) will be left out for convenience.

### 4.6.1 Homogeneous, deterministic simulation

For the 6 different parallel well spacings chosen, simulations were carried out to observe the behaviour of the capture zone under homogeneous assumptions. Of particular importance is the behaviour of the capture zone given the set of aquifer and well parameters used in this simulation. The results (not all) are shown in Figure 4-52.

![Homogeneous capture zones](image)

*Figure 4-52: Homogeneous capture zones for different well spacings parallel to the hydraulic gradient. The well spacings used were 4 (top left), 10 (top right), 20 (bottom right) and 100 (bottom right).*
As the parallel well spacing increases, the down-gradient end of the capture zone becomes thinner. The behaviour of the homogeneous capture zone can be visualised as two separate superimposed capture zones, with half the base extraction rate, being pulled apart in the parallel direction. The total capture zone area is shown in Figure 4-53.

![Homogeneous capture zone area](image)

**Figure 4-53: Homogeneous capture zone area with different parallel well spacings.**

The homogeneous capture zone area decreases fairly linearly for the well spacing range of 0 to 100 in this domain. The homogeneous capture zone is expected to behave as follows: as $t \to \infty$, the capture zone will look like the capture zone for $Q=Q_b/2$ at the down-gradient well, but at the location of the up-gradient well, the capture zone will look like the capture zone of $Q=Q_b$, i.e. two superimposed capture zones of $Q=Q_b/2$ at the location of the up-gradient well.

The homogeneous simulations suggest that the largest capture zone area in a given domain occurs when there is no well spacing, i.e. one well using double the pumping rate. In a limited domain (such as the modelling domain used), the capture zone past a certain up-gradient distance cannot be accounted for and therefore the width (not length) of the capture zone becomes the important factor in driving the total area of capture. This is why the homogeneous capture area in the given domain is highest for no well spacing.
4.6.2 Heterogeneous, stochastic results

10 MC realisations for each well spacing value were carried out using heterogeneous fields with $\sigma_K=3$, $C_L=20m$, $\mu_K=10^{-11}m/s$ and $\nabla h=0.01$. The results for 4 of the 6 simulations are shown in Figure 4-54.

Figure 4-54: Capd for different parallel well spacings through MC analysis. The well spacings used were 4 (top left), 10 (top right), 20 (bottom right) and 100 (bottom right).

Qualitative analysis of the capd plots suggest that the uncertainties in the isolines do not change significantly with increasing well spacings in the range of 4 to 40. This is seen by the similar levels of irregularities in the isolines for all different well spacings and is particularly significant for areas closer to the well. It is possible to conclude from the capd plots that the uncertainty in determining the shape of the capture zone is insensitive to the parallel well spacing.
The uncertainty in determining the size of the capture zone is difficult to determine from visual inspection. Visual analysis suggests that the size of the probabilistic capture areas remain fairly insensitive to the amount of parallel well spacing. Quantitative analyses are required to confirm these observations.

### 4.6.3 Behaviour along central lines

Since there are two pumping wells in this simulation, there is only one shared well line between the two wells. In this case it is the North-South well-line. The behaviour of the capd along the North-South well-line is shown in Figure 4-55.

![Figure 4-55: Behaviour of the capd along the common well-line.](image)

Figure 4-55 shows that as the well spacing is increased from 0, the behaviour of the capd depart from the cumulative normal distribution pattern. The certainty of capture up-gradient and down-gradient of the well display opposite patterns for the well spacings. The larger the well spacing, the smaller the area of uncertainty in the capture zone down-gradient, i.e. more P=0. This is shown by the sharpness of the increase in the graph down-gradient of the well for larger well spacings. However, at up-gradient distances, well spacing lowers the probability of capture and the certainty in the capture zone. This is seen by the departure from normality and the higher levels
of irregularities. No matter what spacing is chosen, the probability of capture at large distances up-gradient stabilises to a similar value.

From Figure 4-55, the effects of adding parallel well spacing to the behaviour of the capd along the North-South line is similar to the effects of increasing the variance. The difference here is the behaviour of any amount of spacing gives a similar effect on the capd, whereas higher $\sigma^2_K$ increases the significance of this effect.

Increasing the parallel well spacing seems to lower the probability of capture for areas located directly up-gradient. This is surprising as it is expected that increasing the spacing in the y direction would increase the probability of capture of an area located further up the same direction.

### 4.6.4 Behaviour of the capd areas P10, P50 and P90

The capture zone areas for P10, P50 and P90 are shown in Figure 4-56 for different parallel well spacings.

![Figure 4-56: P10, P50 and P90 areas for different parallel well spacings.](image)
The areas of P10, P50 and P90 all show a similar trend of a rapidly decreasing area when the wells are spaced in the parallel direction. The decrease in area of P10, P50 and P90 stabilises quickly and remains relatively unchanged for increasing well spacings in the given domain. Since the homogeneous simulations suggests a linear decrease in the capture zone area with increasing parallel well spacing, the result in Figure 4-56 show that there is a departure in behaviour from the homogeneous assumption.

The behaviour of Figure 4-56 is the absolute behaviour of the capds and can again be attributed to two different factors – the expected behaviour via a homogeneous assumption and the change in the levels of uncertainty associated with increasing the parallel well spacing, i.e. the change in ratio of P10 and P90. To isolate the behaviour of uncertainty due to changes in the parallel well spacing, the results are again normalised to the expected homogeneous behaviour. The absolute values for the well spacings are also normalised against a proportion of the heterogeneous correlation scale (isotropic $C_L$) of the hydraulic conductivity in the field. This is done because it is hypothesised that the behaviour of uncertainty for different parallel well spacings are related to the correlation lengths of the soil. The normalised results are shown in Figure 4-57.
Besides from the initial large decrease in P10, P50 and P90, all the probabilistic capture areas remain fairly constant for all parallel well spacings and follow a similar behaviour. This confirms the initial qualitative analysis that the probabilistic areas are insensitive to the amount of well spacing. It can be concluded that when parallel spacing of two wells are increased past a certain value, any further increase in spacing will not change the level of uncertainty in determining the size of the capture zone relative to a homogeneous assumption.

### 4.6.5 Influence of parallel well spacing on the spread

The normalised 80 percent areal spread calculated from the P10 and P90 values are shown in Figure 4-58 for different parallel well spacings.
Figure 4-58 shows that the uncertainty, or relative uncertainty compared to a homogeneous assumption, is highest with no well spacings (one well with double the pumping rate). The absolute level of uncertainty, quantified by the areal spread, remains relatively constant for any amount of parallel well spacings. It is interesting to note, however, that at certain parallel well spacings, the uncertainty can be minimised. In these results this occurs at a spacing of 4 and 20, with 4 giving a slightly lower level of relative uncertainty. In terms of the correlation length (C_L) of hydraulic conductivity, this is 0.2C_L and 1C_L respectively. It is also interesting to see that the relative uncertainty fluctuates slightly in the range of parallel well spacings of 0.2C_L to 2C_L. The fluctuation occurs with a increasing period but stabilises after the parallel well spacing is larger than 2C_L.

4.6.6 Discussion

Qualitative analysis of the capd plots suggest that the uncertainty in determining the shape of the capture zone is insensitive to different well spacings in the range of 4 to 40 (or 0.2C_L to 2C_L).

The absolute size of the probabilistic capture zone (P10, P50 and P90) in a given domain is smaller using two parallel spaced extraction wells with Q_b/2 each in comparison to one single pumping well with the standard pumping rate, Q_b. However,
probabilistic capture areas are relatively less sensitive to the amount of spacing after it is larger than 4 \((0.2C_L)\). This is shown via visual inspection of the capd plots and confirmed via quantitative analysis.

Along the North-South well-line, the behaviour of the capd departs for normality when there is any level of parallel well spacing. The change in behavioural pattern of the capd along this well-line for any well spacing is similar to the effects of increasing the variance. However, once again, the amount of spacing does not seem to influence the behavioural pattern of the capd and the probability of capture for particles located at large distances both down-gradient and up-gradient of the wells.

The probability of capture for a particle located at a large distance directly up-gradient of the pumping wells are lower using two parallel spaced wells compared to using a single well. This can be explained by the fact that the two wells use half the pumping rate of the one well scenario. From the one well simulation carried out with different extraction rates, we know that the probability of capture for particles located at a large distance directly up-gradient of the well is related to the extraction rate. The lower the extraction rate, the lower the probability of capture. A particle will generally take more time to reach the well for lower extraction rates and therefore have a higher probability of being caught in areas of low hydraulic conductivity. This is why a particle will ‘feel’ the heterogeneity of hydraulic conductivity more for lower extraction rates and is explained in the previous one well simulation.

At large distances directly up-gradient, the probability of capture is therefore influenced by two conflicting factors. Firstly, it is expected that placing a second well in a certain direction should increase the probability of capture of a particle in that direction. This fundamental relationship is obvious from the fact that areas located closer to an extraction well should have a higher probability of capture. The second factor, which conflicts with the first factor, is the fact that the wells used in the two well simulations have half the pumping rate of the one well scenario. This means heterogeneity will have a higher effect in the capture zones of the two wells with half the pumping rate. This causes the probability of capture for large distances directly up-gradient of the well to decrease. The lower probability of capture directly up-gradient, as seen in the results from the North-South well-line, suggests that in this
simulation the effects of a lower extraction rate over-shadows the fundamental expectation in heterogeneous formations. This, of course, depends on the heterogeneity of the field and the absolute extraction rate used.

Even though the absolute size of the capture zone area in a given domain becomes smaller when using two parallel spaced wells with $Q_b/2$ compared to one well with $Q_b$, the certainty in the capture zone is higher for two parallel spaced wells. This is shown via the large drop in the 80 percent areal spread. Any amount of parallel well spacing will give higher certainty in the capture zone compared to no spacing, but at certain spacings the spread can be minimised. In this simulation, this spacing corresponded to $0.2C_L$ and $1C_L$. It is hypothesised that the parallel well spacing which minimises uncertainty is related to the estimated correlation length of hydraulic conductivity of the field. Further simulations using different correlation structures need to be carried out to confirm this.

The location of the capture zone, via analysis of P50, follows a similar pattern as P10 and P90. The location in a given domain shrinks rapidly when the well spacing increases from 0 to $0.2C_L$. It then stabilises and remains insensitive to any further increases in well spacings. This behaviour contradicts the linear decreasing expectation from homogeneous assumptions. This is because even though the capture zone in a given domain is expected to shrink via the homogeneous assumption, the associated lower level of uncertainty of using two wells (seen in the areal spread) keeps the P50 area from decreasing. The expected decrease in size is thus offset by a higher level of certainty in the capture zone.

Since the spread remains fairly constant for any level of spacing, the important conclusion here is that even though a single well is expected to produce a larger capture area (in both homogeneous and heterogeneous formations), two parallel spaced wells with half the pumping rate will increase the level of certainty in the capture zone size regardless of the amount of spacing - that is, relative to the homogeneous expectation. This result should increase in significance with increasing heterogeneity (variance) in hydraulic conductivity.
Based on the results from this simulation, the behaviour of the capture zone in heterogeneous formations is as follows:

- The absolute size of the capture zone is expected, and is confirmed to decrease with two parallel spaced wells with $Q_b/2$ compared to one well with $Q_b$;
- The level of uncertainty in determining the shape of the capture zone remain relatively unchanged for different parallel well spacings larger than 4 ($0.2C_L$);
- The probability of capture of a particle at large distances directly up-gradient of the well depend on two factors: the extraction rate relative to the heterogeneity and the up-gradient placement of the second well. If the first factor dominates $P_{\text{capture}}$ will be smaller due to high $\sigma_K^2$ and low $Q$;
- Any amount of parallel well spacing will result in higher certainty in the size of the capture zone compared to one well;
- The level of uncertainty for two parallel spaced wells is fairly insensitive to the amount of spacing, but can be minimised at certain spacings. The results here suggest a spacing of 0.2CL or 1CL will minimise the uncertainty;
- The location of the capture zone shrinks when parallel well spacing increase from 0 to 4 (0.2CL). It then becomes stable and remains unchanged for any amount of spacing.

### 4.7 Dual well simulation – Varying well spacing perpendicular to the hydraulic gradient

The aim of this simulation is to quantify the effects of changing the perpendicular well spacing on the capd. The main focus is to determine a general relationship between the distance in perpendicular well spacing and the resulting uncertainty within the capture zone. The influence of perpendicular well spacing on the size, shape and location of the resulting capture zone can then be quantified by analysing the results. The results in this section will again be compared to the solutions derived from homogeneous assumptions. This will show the level of uncertainty relative to the amount of deviation from a homogeneous assumption.

The simulations used a perpendicular well spacing of 0, 4, 10, 20, 40 and 100 (all in meters). The well spacings corresponded to 0, 1/5, ½, 1, 2 and 5 times the
heterogeneous correlation structure of the field. The extraction rate used was half the extraction rate of the single well simulations, i.e. 0.01 m³/s. This was chosen so a direct comparison can be seen via using the same total extraction rate (0.02 m³/s). The standard well location was at x=250, y=400 for the one well simulations. In this simulation, the wells’ locations are shown in Table 4-1.

Table 4-1: Locations of the two wells for each simulation

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Extraction well 1 (x,y)</th>
<th>Extraction well 2 (x,y)</th>
<th>Perpendicular distance</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(250,400)</td>
<td>(250,400)</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>(248,400)</td>
<td>(252,400)</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>(245,400)</td>
<td>(255,400)</td>
<td>10</td>
</tr>
<tr>
<td>4</td>
<td>(240,400)</td>
<td>(260,400)</td>
<td>20</td>
</tr>
<tr>
<td>5</td>
<td>(230,400)</td>
<td>(270,400)</td>
<td>40</td>
</tr>
<tr>
<td>6</td>
<td>(200,400)</td>
<td>(300,400)</td>
<td>100</td>
</tr>
</tbody>
</table>

In total, 10 heterogeneous fields were created for each of the well spacing values. This resulted in a total of 60 separate deterministic simulations being used for this section. The MC analysis produced 6 stochastic capds.

All other parameters were kept constant at their standard values except for the pumping rate of each well was Qb/2 and the well spacing, i.e. σ²K = 3, Cₗ = 20, \( \nabla h = 0.01 \) and \( \mu_k = 10^{-11} \) m/s. The units for the spacings (in meters) will be left out for convenience.

4.7.1 Homogeneous, deterministic simulation

For the 6 different perpendicular well spacings chosen, simulations were carried out to observe the behaviour of the capture zone under a homogeneous assumption. The results (not all) are shown in Figure 4-59.
Figure 4-59: Homogeneous capture zones for different well spacings perpendicular to the hydraulic gradient. From left to right, the top row has spacing of 4, 10 and 20 while the bottom row has 40 and 100.

As the perpendicular well spacing increases, the down-gradient end of the capture zone begins to split up. The behaviour of the homogeneous capture zone can once again be visualised as two separate superimposed capture zones, with half the base extraction rate, being pulled apart in the perpendicular direction. The total capture zone area is shown in Figure 4-60.

Figure 4-60: Homogeneous capture zone area with different perpendicular well spacings.
In this domain, the homogeneous capture zone area increases slightly as the well spacing increases from 0 to 20. After 20, the capture zone area decreases and stabilises to the area equivalent to two separate unconnected capture zones produced by \( Q = Q_b / 2 \). The initial increase in the capture zone area is due to the effects of superimposition of the capture zones of the two wells. This results in a wider capture zone when they are connected in comparison to the sum of the widths of the capture zones when they are separate. In a limited domain (such as the modelling domain used), the capture zone past a certain up-gradient distance cannot be accounted for and therefore the width (not length) becomes the important factor in driving the area of capture.

Given an equal total extraction rate, the homogeneous simulations suggest that the largest capture zone area in a given domain occurs when the wells are spaced 20m apart. Note however the scale of the graph starts at 70000. In absolute terms, the capture zone area calculated under a homogeneous assumption for this domain actually remains fairly constant.

### 4.7.2 Heterogeneous, stochastic results

10 MC realisations for each well spacing value were carried out using heterogeneous fields with \( \sigma_K = 3 \), \( C_L = 20 \)m, \( \mu_K = 10^{-11} \)m/s and \( \nabla h = 0.01 \). The results are shown in Figure 4-61.
Qualitative analysis of the capd plots suggest that the uncertainties in the isolines do not change significantly in the range of 4 to 10. This is seen by the similar levels of irregularities in the isolines. However, when the spacing is increased past 10, the irregularities seem to increase and are especially obvious for a spacing of 40 and 100.

The uncertainty in determining the size of the capture zone is difficult to determine from visual inspection. From the capd plots, the area of uncertainty (i.e. $0<P<1$) seems to be larger for perpendicular spacings of 40 and 100. The smallest area of uncertainty occurs for well spacing of 10 while a spacing of 4 and 20 displays a similar, but slightly higher area of uncertainty. This has to be confirmed via quantitative analyses.
4.7.3 Behaviour along central lines

Since there are two pumping wells in this simulation, there is only one shared well line between the two wells. In this case it is the West-East well-line. The behaviour of the capd along this well-line is shown in Figure 4-62.

![Behaviour of the capd from West to East (x axis at y=400)](image)

Figure 4-62: Behaviour of the capd along the common well-line.

Figure 4-62 shows that as the perpendicular well spacing is increased, the capd distribution along this well-line widens and slowly becomes two separate normal distribution type curves. The capd behavioural pattern as the spacing increases can thus be described via two normal distributions being pulled apart. However, unlike the description of the capture area under a homogeneous assumption, the principle of superimposition does not hold here as the graph measures probability. The capd widens (more 0<P<1) as well spacing is increased before separating into two curves.

From Figure 4-62, it can be seen that a spacing of 100 has the highest area of uncertainty (0<P<1). All other well spacings between 4 and 20 share a fairly identical area of uncertainty, with 20 being slightly higher. This suggests that the area of uncertainty is generally increasing with increasing perpendicular spacing, but the details between the spacing of 4 to 20 are not quite visible. Further quantitative analysis is needed to confirm this.
4.7.4 Behaviour of the capd areas P10, P50 and P90

The capture zone areas for P10, P50 and P90 are shown in Figure 4-63 for different perpendicular well spacings.

Figure 4-63: P10, P50 and P90 areas for different perpendicular well spacings.

Figure 4-63 shows that when the perpendicular spacing is increased from 0 to 4, both P50 and P90 decrease. P10 remains fairly stable. Increasing the spacing from 4, P10 and P90 display opposite trends. From 4 to 10, P90 increases then decreases for any spacings higher than 10. P10 decreases from 4 to 10 and then generally increases for spacings above 10.

The behaviour of Figure 4-63 is the absolute behaviour of the capds and can again be attributed to two different factors – the expected behaviour via a homogeneous assumption and the change in the levels of uncertainty associated with increasing the perpendicular well spacing. Since the behaviour of the P10 and P90 areas differ from the expected homogeneous behaviour, we know that the amount of well spacing influences the uncertainty in the capture zone. To isolate this effect the result is again normalised with the expected homogeneous capture area and the correlation structure. This is shown in Figure 4-64.
Figure 4-64: P10, P50 and P90 areas normalised against the homogeneous capture area. Well spacing is shown as a multiple of hydraulic conductivity's correlation length.

Since the homogeneous capture areas in this domain remain fairly constant for well spacings of 0 to 100 (Section 4.7.1, Figure 4-60), the normalised results show hardly any difference in behaviour. The behaviour of the P10, P50 and P90 areas are thus due mainly to the effects of changing the perpendicular well spacing on the level of uncertainty. The area of certainty remains fairly constant for any amount of well spacing and slowly decreases with large magnitudes of increase in well spacing. An important observation is that a peak occurs at spacing of 10 (0.5C_L). Even though the P10 area generally increases for higher well spacings, a corresponding minimum value occurs at a spacing of 10. This suggests that the level of uncertainty in the size of a capture zone generally increases with larger perpendicular well spacings but will correspond to a minimum for a certain spacing (0.5C_L in this case).

P50, representative of the median isochrone and the location of the capture zone, remains fairly constant for any perpendicular spacing in the range of 0 to 40 (0-2C_L). It then decreases slightly compared to the homogeneous capture area when the well spacing increased for a larger range due to increases in uncertainty.
4.7.5 Influence of horizontal well spacing on the spread

Figure 4-65 shows the normalised 80 percent areal spread for different perpendicular well spacings.

![Figure 4-65: Normalised areal spread against parallel well spacing.](image)

From Figure 4-65 it can be seen that the normalised areal spread follows a fluctuating pattern but generally increases with larger perpendicular well spacings. The important feature of Figure 4-65 is that the areal spread is minimised at a certain well spacing (0.5C_L in this case). This suggests that when two wells are used (or one well with double the pumping rate, i.e. 0 spacing), a perpendicular well spacing of 0.5C_L in a heterogeneous formation corresponds to the capture zone behaving most similarly to a homogeneous assumption. This, however, should depend on other parameters such as Q, C_L, σ^2_K and V h.

4.7.6 Discussion

Qualitative analysis of the capd plots suggest that the uncertainty in determining the shape of the capture zone is insensitive to the perpendicular well spacings in the range of 0 to 10 (or 0 to 0.5C_L). However, a spacing larger than 10 (0.5C_L) seems to increase the uncertainty in the capture zone shape delineation. This can be explained
by the fact that lower extraction rates are more affected by heterogeneity. As the wells are spaced apart, the effects of the lower extraction rate of the individual wells (Q_b/2) become more visible. The effects of heterogeneity may not be felt in the capture zone when the wells are still close together (spaced 4-10m or 0.2C_L-0.5C_L). This results in the higher irregularities observed in the isolines, meaning an increase in uncertainty in determining the shape of the capture zone with spacings above 10. The point where the lower extraction rate affects the certainty in shape delineation should depend on the absolute extraction rate relative to the heterogeneity (variance) of the field.

Along the common well-line, the capd distribution widens and slowly becomes two separate normal distribution curves without superimposing the probability of capture. The capd behaviour moving from West to East can thus be described as widening (more 0<P<1) before separating into two curves.

The absolute size of the probabilistic capture zone (P10, P50 and P90) in a given domain is relatively constant regardless of the perpendicular well spacing. This is seen in the behaviour of P10, P50 and P90 with different spacings. However, P10 and P90 is at a minimum and maximum (respectively) for a certain perpendicular spacing suggesting that uncertainty can be minimised by strategically spacing the wells. For the parameters used in this simulation, the point corresponded to half the heterogeneous correlation length. This can be confirmed by the visual capd plots and the calculation of the areal spread.

The areal spread shows that uncertainty in the size of the capture zone can be minimised by placing two wells at a distance of 0.5C_L apart. This can be explained by the factors that drive uncertainty in the heterogeneous formation. Firstly, we can assume the behaviour of the probabilistic capture areas are driven by both the homogeneous expectation and the changes in the level of uncertainty of different perpendicular well spacings. The level of uncertainty, however, is driven by both the well spacing and the ratio between Q and σ_K^2. If Q is small relative to σ_K^2, the level of uncertainty will be higher due to the increasing effects of heterogeneity. Conversely, placing two perpendicular spaced wells should increase the certainty of capture since fundamentally the probability of capture is higher closer to the well. At a certain well spacing, the higher effects of heterogeneity felt by a smaller Q (Q_b/2 compared to one
well using $Q_b$) may be minimised due to the overlapping capture zones of the two separate wells. Also, at this point, the increase in certainty by using two separate wells will also be felt and thus correspond to a minimum level of uncertainty. For this simulation, this point occurred at $0.5C_L$. When the spacing is further increased, the uncertainty resulting from the lower $Q$ begins to overshadow the higher level of certainty from placing two wells and can be seen by the increase in areal spread for larger perpendicular well spacings. The spacing that minimises uncertainty should be dependent on other parameters, the most important being the correlation length and the ratio of $Q$ to $\sigma_K^2$. Further simulations are needed to confirm this hypothesis.

The important conclusion here is that when two perpendicular spaced wells are used to minimise uncertainty in the capture zone, the distance between the wells needs to be carefully calculated. This is because the areal spread is considerably larger for higher perpendicular spacings (higher than $2C_L$) in comparison to the range of $0-2C_L$. Although there is a certain well spacing that minimises uncertainty ($0.5C_L$ here), if field measurements of parameters are unavailable or inaccurate, it may be better to place one extraction well that has double the pumping rate. Unlike the previous simulation where any amount of parallel well spacing gave higher levels of certainty in the capture zone compared to using one well, perpendicularly spaced wells may create higher levels of uncertainty if the chosen spacing is too high.

Based on the results from this simulation, the behaviour of the capture zone in heterogeneous formations is as follows:

- The absolute size of the capture zone is expected remain fairly constant (slight decrease in the domain) with increasing perpendicular well spacing using a homogeneous assumption. Probabilistic areas shows that it remains fairly constant in a certain range ($0-2C_L$);
- The level of uncertainty in determining the shape of the capture zone remain relatively unchanged for a certain range ($0-0.5 \ C_L$) but increases with higher well spacings ($>0.5C_L$);
- The capd behaviour moving from West to East can be described as a widening normal distribution before separating into two separate normal distributions for increasing perpendicular spacings;
• The areal spread shows that uncertainty in the size of the capture zone can be minimised by placing two wells at a certain perpendicular distance apart (0.5C_L) and is likely to be dependent on C_L and the ratio of Q to σ^2_K;

• Unlike two parallel spaced wells, a single well with double the extraction rate may give higher levels of certainty in the capture zone compared to two highly perpendicularly spaced wells.
Chapter 5

Summary and Conclusions
5 Summary and conclusions

Different aquifer and well properties that fundamentally affect the capture zone include the hydraulic conductivity, the hydraulic gradient, the well pumping rate, the location of the pumping well and the number of pumping wells. These properties have been extensively studied in the past and analytical formulations exist in determining their effects on the well capture zone. However, these formulations are based on the assumption of homogeneity and thus limiting their applications in the field.

Stochastic analysis and geostatistics can be used to simulate heterogeneity in the field. Compared to the assumption of homogeneity, stochastic analysis can provide a more “honest” analysis of the capture zone via descriptions of the associated uncertainty. The resulting capd form an important part of risk evaluation for the development of groundwater source protection policy - as risk analysis is based on the probability of occurrence. An increasing number of studies over recent years have adopted this method of approach due to the increases in computational efficiency to deal with large numbers of Monte Carlo realisations. Past stochastic capture zone studies, however, have focused solely on the effects of the variance and correlation structure of heterogeneity on the extent of uncertainty about the location of a capture zone. There are no stochastic studies carried out to investigate the effects on uncertainty in the capture zone due to changing fundamental well and aquifer properties that determine the capture zone in homogeneous formulations.

The results from the previous chapter used a heterogeneous stochastic approach to investigate uncertainties associated with the fundamental well and aquifer properties that determine the capture zone in homogeneous formulations. This provides a link between past studies under a homogeneous assumption and the stochastic studies of heterogeneous aquifers. In determining the location of the capture zone in heterogeneous formations, the median isochrone resulting from the MC analyses was adopted due to its insensitivity to outliers. The uncertainty in delineating the capture zone was qualitatively described via the probability distribution plots (capds) and the behaviour along the virtual well lines. Quantitative analyses of P10 and P90 resulted
in a description of the absolute uncertainty in the capture zone and deviation from the
homogeneous assumption in appropriate cases.

As previous stochastic capture zone studies are centred on $\sigma^2_K$ and $C_L$, an important
conclusion from this study is that uncertainty within the capture zone in
heterogeneous conditions is not only affected by these two factors. In a two
dimensional confined aquifer at steady state, the results are summarised in Table 5-1.
Table 5-1: Summary of results for different aquifer and well properties

| Aquifer or well property | Summary of Results (for t→∞) | Normalised areal spread and uncertainty (deviation from the homogeneous capture zone area) $s^2_{\text{capd}}=[1/4(P10-P90)]^2$
<table>
<thead>
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<tbody>
<tr>
<td>Homogeneous capture zone area in the domain</td>
<td>Heterogeneous capture zone area in the domain (P50)</td>
<td>$σ^2_{K}$ produces a single, deterministic capture zone</td>
</tr>
<tr>
<td>$C_L$</td>
<td>Homogeneous aquifer with random K (for $C_L→∞$). Solution can be solved analytically resulting in a smooth capd dependent on $μ_K$, $Q$, $∇h$ and $σ^2_{K}$.</td>
<td>Decreases with increasing $C_L$ in the range $5&lt;C_L&lt;40$. When $C_L&gt;100$, capture area increases due to lower levels of uncertainty as the problem approaches homogeneity ($C_L→∞$).</td>
</tr>
<tr>
<td>$C_{LX}:C_{LY}$</td>
<td>-</td>
<td>Expands with higher $C_{LX}:C_{LY}$ ratio, i.e. higher $C_L$ perpendicular to $∇h$. $C_{LX}:C_{LY}$</td>
</tr>
<tr>
<td>$\nabla h$</td>
<td>Capture zone area is inversely proportional to $\nabla h$ (i.e. Area=$C/\nabla h$).</td>
<td>Absolute capture zone area follows the behaviour of the homogeneous capture zone area sharing an inversely proportional relationship with $\nabla h$. However, it shrinks relative to the homogeneous capture zone with increasing $\nabla h$ (for $\nabla h&gt;0.03$) due to increasing uncertainty.</td>
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<tr>
<td>$Q$</td>
<td>Capture zone area increases linearly with increasing $Q$.</td>
<td>Absolute area increases linearly with increasing $Q$. However at small $Q$, the capture zone area is much smaller than the homogeneous capture zone due to high uncertainty. As $Q$ increases, the capture area increases faster than the homogeneous capture area due to increases in certainty. The rate of Normalised areal spread decreases at a decreasing rate with increasing $Q$. It can be related to $Q$ via the equation $f(x)=a+b.x^{-1}$. The constant ‘$a$’ is proven to be directly related to $\sigma^2_K$. The constant ‘$b$’ is most likely dependent on other parameters such as $\nabla h$, $Q$, $\mu_K$ and $C_L$ but need further experimentation. This means the capture zone area diverts from the homogeneous assumption via the above equation.</td>
</tr>
<tr>
<td>Well Spacing</td>
<td>Parallel Well Spacing</td>
<td>Perpendicular Well Spacing</td>
</tr>
<tr>
<td>-------------------------------</td>
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<td>-----------------------------</td>
</tr>
<tr>
<td>Increase decreases with higher Q.</td>
<td>Decreases in a linear pattern with increasing spacing.</td>
<td>Remains fairly constant for increasing spacing.</td>
</tr>
<tr>
<td>Decreases when spacing is increased from 0 to $0.2C_L$ in the given domain. It then remains fairly stable for any further increase in spacing and does not decrease linearly like the homogeneous capture area due to higher levels of certainty.</td>
<td>Remains fairly constant when spacing is increased from 0 to $2C_L$. When the spacing is higher than $2C_L$, the capture area decreases both in absolute size and relative to the homogeneous capture area due to increasing uncertainty.</td>
<td>The normalised areal spread shows that certain values of spacing results in higher uncertainty in the capture zone compared to a single well with double the pumping rate (i.e. spacing=0). However, spacing can be strategically chosen to minimise uncertainty, i.e. give the smallest deviation from the homogeneous assumption. This occurred for a spacing of $0.5C_L$.</td>
</tr>
</tbody>
</table>

*Note: The normalised areal spread shows that any amount of well spacing in the range of $0.2C_L$ to $5C_L$ give higher certainty in the capture zone compared to no spacing. A spacing of $0.2C_L$ and $1C_L$ resulted in the highest level of certainty, i.e. smallest deviation from the homogeneous assumption.*
5.1 Applications to the field and limitations

The results from Table 5-1 can be directly applied to groundwater protection applications through improving the accuracies associated with probability risk assessments. The quantified relationships between the level of uncertainty in the capture zone and the associated parameter can be used in risk analysis to better describe vulnerability. For example, increasing $\nabla h$ results in a smaller capture zone and increases the uncertainty in capture zone delineation. From the results of this study, the capture zone calculated under heterogeneous conditions deviates linearly from the homogeneous capture zone as $\nabla h$ increases, i.e. a linearly increasing normalised spread. Therefore if the measured $\nabla h$ in the protected quantity (the capture zone area) is small, a linear relationship can be used to factor in an additional level of associated risk.

The results from the dual well simulations shows there is a certain well spacing that can minimise uncertainty within the capture zone and is dependent on the aquifer and well properties, most importantly the correlation length. Field practitioners can thus strategically space wells to minimise uncertainty in capture zone delineation. They can be certain that any amount of spacing parallel to $\nabla h$ will result in higher levels of certainty under heterogeneous formations.

However, care must be taken in application of the derived relationships due to the limitations of the simulations. There are errors associated with MC analyses and limitations in representing hydraulic conductivity with a natural-log normal distribution as discussed in chapter 2. Also the scale of consideration is important as this study averages the thickness of an aquifer. The assumptions of a confined aquifer at steady state also means that the results derived in this study have no additional recharge to the aquifer, is under fully saturated conditions and occur after a large elapsed time scale. Other important factors discussed in chapter 2 that need consideration include uniformity in $\nabla h$, effective porosity and hydrogeological conditions at aquifer boundaries.
5.2 Recommendations for future work

The relationships derived in this thesis presents large opportunities for future research into quantifying the level of uncertainty in capture zones associated with certain aquifer and well properties. Further simulations can directly expand the scope of this study by determining the coefficients that define the relationship between uncertainty and the associated aquifer or well property. For example, the results showed with increasing Q the heterogeneous capture zone area deviates from the homogeneous capture zone area. This deviation can be quantified via the equation \( a + b \cdot Q^{-1} \). Using a dual variable methodology, this study found the coefficient ‘a’ to be directly dependent on \( \sigma^2_k \). Further dual variable simulations can be carried out to determine which parameters determine b. Due to the many variables that may affect uncertainty in the capture zone, there are a large number of available cross examination tests that can be carried out between two variables to determine the coefficients.

For the dual well simulations, further simulations with different \( \sigma^2_k \) and \( C_L \) values can confirm whether or not uncertainty is always minimised for a parallel and perpendicular well spacing of \( 0.2C_L \) and \( 0.5C_L \) respectively. Further studies can be carried out with different combinations of extraction and injection well patterns to determine a relationship between uncertainty, the number of extraction and injection wells and the location (or spacing) of the wells. This can result in certain recommended formations in well patterns that minimise uncertainty in the capture zone under heterogeneous conditions.

Following the methodology set up in this study, transient simulations can also be carried out to study the effects of uncertainty within the capture zone in terms of the elapsed time. Also, using the same methodology, higher number of MC realisations can be used to confirm the derived relationships in this thesis and rule out convergence errors. The methodology in this study can also be adopted to simulate other heterogeneous aquifer properties with unpredictable spatial variability. This includes recharge, the saturated thickness, the effective porosity and the hydrogeological conditions at aquifer boundaries that may influence the distribution of hydraulic head. Uncertainty in the capture zone resulting from the heterogeneity of these parameters can then be quantifiable.
6 References


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