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# GROUNDWATER MODELING AND MANAGEMENT

# USING

# THE FINITE ELEMENT METHOD AND EVOLUTIONARY OPTIMISATION TECHNIQUES

**By**

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**Dedicated**
**to**
**my wife and kid(s)**
**for their**
**love, understanding, and encouragement**

## Statement of Originality

This work contains no material which has been accepted for the award of any other degree or diploma in any university or other tertiary institution, and to the best of my knowledge and belief, contains no material previously published or written by any other person, except where due references is made in the text.

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# Synopsis

For realistic modeling of a groundwater system, to problems namely: (1) the forward problem (simulation) and (2) the inverse problem (calibration) must be solved. The forward problem predicts the unknown system states given the known system parameters and boundary conditions. The inverse problem determines the unknown physical parameters of the system by fitting observed system states. The inverse problem must first be solved to determine the appropriate model structure and model parameters in order to obtain reliable results from the forward solution. Solution of an inverse problem or a management decision problem requires the use of optimisation techniques. For the past two decades, the techniques that have been used for such problems have been blocked by several inherent difficulties. Firstly the solution of the inverse problem may be nonunique and unstable as a result of observation errors. Secondly, the quality and quantity of observation data are insufficient. Thirdly, the model structure error which is difficult to estimate, dominates other errors. Within the inverse model itself, the computation of derivatives as required by the gradient-based techniques also introduce the problem of ill-conditioning and instability for highly nonlinear problems and very sensitive parameters.

The present research study was initiated with the objective of using evolutionary techniques instead of the gradient-based methods to solve the optimisation problems embodied in both management and inverse models. The research study was completed in two phases. The work accomplished during the first phase of the study included the development of an inverse model for the identification of groundwater flow and solute transport parameters through the use of the shuffled complex evolutionary technique with finite element models developed to solve two- and three-dimensional problems. The resulting inverse model was tested extensively with field pumping test, synthesised data and corrupted synthesised data. The results of the test indicated that the shuffled complex

evolutionary technique of optimisation was robust, efficient, and effective, and could serve as a useful alternative to the more traditional gradient-based methods. The attractiveness of the technique lies in the fact that it performs its search without the need for computation of derivatives; a feature that makes the shuffled complex evolution superior to the gradient-based methods in the event of highly nonlinear problems and parameter sensitivity and interaction. A critical test carried out to investigate the weakness of the shuffled complex evolutionary technique indicated that the population of points in the search space must be well selected in order to achieve a more reliable and cost effective solution.

The second phase of the research study was the development of management-decision model for the optimisation of pollutant extraction from contaminated aquifers using the genetic algorithm evolutionary technique. Once again, this optimisation technique was linked with a finite element numerical model. An additional technique developed and incorporated into the standard genetic algorithm model was a time-variation approach that allowed the location and numbers of pumping rates to vary as the contaminant plume moves along with time. This precaution was taken to avoid redundancy of extraction wells (an hence excessive remedial costs) as the plumes move away from their original location with the progress of time during the forward simulation process. A theoretical analysis using both the standard genetic algorithm and the time-variation technique indicated that the latter was more efficient resulting in about 27% and 16% cost savings respectively, for both one- and two-dimensional potential arrangements of extraction wells.

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# Chapter 1

# Introduction

## 1.1 Why this Research Project

Groundwater constitutes an important component of many water resource systems; supplying water for domestic use, for industry and for agriculture. Management of a groundwater system, or a system of aquifers means making such decisions about the total quantity of water drawn annually, and if remediation is required, the optimum number, pumping rate, and location of extraction wells for a cost effective clean up operation. Also equally important are decisions related to the quality of groundwater being used for domestic and industrial purposes. In fact, the quantity and quality problems can not be separated.

In many parts of the world, the increased withdrawal of groundwater has caused continuously deteriorating quality, causing much concern to both suppliers and users. In addition to the general groundwater quality aspects, public attention has been focused on groundwater contamination by hazardous industrial waste, by leachate from land fills, by oil spills, and agricultural activities such as the use of fertilisers, pesticides, and herbicides, and by radioactive waste in repositories located in deep geological formations. In all these cases, management means making decisions to achieve goals without violating specified constraints. In order to enable the planner, or the decision maker, compare alternative models of a management decision and to ensure that constraints are not being violated, a

tool is needed that will provide information about the response of the system (the aquifer) to various alternatives. Good management requires the ability to forecast the aquifer's response to planned operations such as pumping, recharging, extraction of contaminants etc. This response may take the form of changes in water level, changes in water quality, or land subsidence.

Any planning, mitigation, clean up operation, or control measures, once contaminant has been detected in the saturated or unsaturated zone, requires the prediction of the path and the fate of the contaminants in response to the planned activities. Any monitoring or observation network must be based on the anticipated behaviour of the system. The necessary information about the response of the system is provided by a model that describes the behaviour of the system under consideration in response to excitation. Such anticipated behaviour can be predicted if parameters governing the response of the system can be estimated. The model required for such predictions may take the form of a well posed mathematical problem, that could be reduced to a set of algebraic equations using numerical formulation techniques. Such tools are referred to as numerical models.

During the past thirty years or so, the techniques of numerical modelling have been extensively used in the study of groundwater resources management, seawater intrusion, aquifer remediation, and other problems related to groundwater. To build a model for real groundwater systems, two problems, the forward (simulation) and its inverse (calibration) must be solved. The former predicts unknown system states by solving appropriate governing equations, while the latter determines the unknown physical parameters and other conditions of the system by fitting observed system states. To solve the forward problem, one must first find the appropriate model structure and parameters. Unfortunately, studies on these two problems have never been in balance. The study of the forward problem has developed rapidly. While one can accurately simulate three-dimensional multicomponent transport in multiphase flow without any essential difficulties, the study on the inverse problem is still limited to consideration of very simple problems. The model quality can not

be improved by increasing the accuracy of the forward solutions alone. The progress of the inverse solution techniques is blocked by several inherent difficulties. First, the inverse problem is often ill-posed, implying that its solution may be non-unique and unstable with respect the observation errors. Second, the quantity and quality of observation data are usually insufficient. Third, the model structure error, which is difficult to estimate, often dominates other errors. Therefore in the presence of all these difficulties a more robust, efficient and effective technique of solving the inverse problem is required.

Part of the success of modelling the forward problem is due to the advancement of modern technology in computers. Today even complex coupled three-dimensional problems of flow and solute transport can be accurately simulated on modern computers within some few seconds. Sophisticated numerical models have been designed that could predict responses such as head, pressure, temperature, velocities, concentration etc. in groundwater systems. However, management decision processes are not just the mere prediction of these response parameters. In as much as decision-makers are eager to know the extent to which an aquifer has been polluted, they may also be interested in knowing the efficient and cost effective method of cleaning up (or extracting) the contaminated aquifer. Some of these efficient and cost effective methods of cleaning up a contaminated aquifer requires the optimum selection of the number, location, pumping rate, time of operation of extraction wells etc. This information is usually missing from most sophisticated groundwater numerical models of flow and solute transport available today.

## 1.2 Research Objectives

From the above introduction, development of any numerical model for groundwater system management must include facilities that will render the model applicable to the following cases: (1) identification of the system formation parameters for the forward model simulation and (2) identification of optimum extraction well locations and pumping rates for possible clean up of a contaminated aquifer. The second of these two, although very important in decision-making, is rarely embodied in flow and solute transport numerical models. In view of these the objectives of the research study are as follows:

- To design a methodology based on the shuffled complex evolutionary process rather than gradient-based techniques, for the identification of aquifer formation parameters in the context of both two- and three-dimensional flow and solute transport numerical models.

- To develop a management model for optimum design of a system clean up operation with respect to the number, location, and pumping rates of extraction wells using the genetic algorithm evolutionary technique of optimisation.

## 1.3 Thesis Format

The thesis is structured in the following form:

### Chapter 2

A comprehensive review of the techniques that have been adopted to date for the inverse problems of parameter identification and management decision models.

### Chapter 3

A brief introduction of the methodology adopted for the execution of the proposed research work.

### Chapter 4

Presentation of the governing equations of the flow and solute transport models, their formulation into a system of algebraic equations by the finite element method, and the appropriate solution techniques used to solved the algebraic equations.

### Chapter 5

Presentation of the genetic algorithm technique for the optimisation of extraction processes and the shuffled complex evolution for the inverse problem of parameter identification.

### Chapter 6

Tests of the accuracy of the inverse model using analytical models with field data and synthetic data. Evaluation of the predictive accuracy of the two- and three-dimensional solute transport numerical models using appropriate analytical models.

## Chapter 7

Application of the inverse model to the identification of aquifer formation parameters using both synthetic and corrupted synthetic data in the context of two- and three-dimensional numerical flow and solute transport.

## Chapter 8

Application of the extraction management model to a hypothetical field-scale problem.

## Chapter 9

Presentation of the conclusions, recommendations and research contributions from this research project.

# Chapter 2

# Review of Inverse and Management Decision Models

## 2.1 Introduction

This chapter reviews inverse and forward techniques that have been adopted in water resources management in the past. In this regard such issues as strengths and weaknesses of the various methodologies are addressed where necessary. The review also mentions some current modelling techniques that have been used. The two evolutionary techniques (1) the genetic algorithm and (2) the shuffled complex evolution proposed to be used in this research project are briefly introduced.

## 2.2 The Inverse Problem

The problem of parameter estimation in distributed parameter systems has been studied extensively during the last two decades. The term *distributed parameter system* implies that the response of the system is governed by a partial differential equation and parameters embedded in the equation are spatially dependent. The inverse problem of parameter estimation (or identification) concerns the optimal determination of the

parameters by observing the dependent variable collected in the spatial and time domains. The number of observations are finite and limited whereas the spatial domain is continuous. For an inhomogenous aquifer the dimension of the parameter is theoretically infinite. In practice, spatial variables are approximated by a finite difference or finite element scheme while the aquifer system is subdivided into several sub-regions with each sub-region characterised by a constant parameter. The reduction of the number of parameters from the infinite to the finite dimensional form is called parameterisation.

Two types of errors are associated with the inverse problems: (1) the system modelling error, as represented by a performance criterion, and (2) the error associated with parameter uncertainty. An increase in parameter dimensions (the number of unknown parameters associated with parameterisation) generally improves the system modelling error but increases the parameter uncertainty. The optimum level of parameterization depends on the quality and quantity of observed data.

## 2.3 Classification of Inverse Methods

Various techniques have been developed to solve the inverse problem of parameter identification. *Neuman* [1973] classified the techniques as either *direct* or *indirect*. The direct approach treats the model parameters as dependent variables in a formal inverse boundary value problem. The indirect approach is based on an output error criterion where an existing estimate of the parameters is iteratively improved until the model response is sufficiently close to that of the measured output. In a survey paper by *Kubrusly* [1977] on distributed parameter system identification, he classified the identification procedures into three categories : (1) direct method, which consists of those methods that use optimisation techniques directly to the distributed (infinite dimensional) model, (2) reduction to a lumped

parameter system, which consists of those methods that reduce the distributed parameter system to a continuous or discrete-time lumped parameter system which is described by ordinary differential equations or difference equations, and (3) reduction to an algebraic equation, which consists of those methods that reduce the partial differential equation to an algebraic equation.

There are only two types of error criteria that have been used in the past in the formulation of the inverse problem for a distributed parameter system. *Chevant* [1979b] classified the identification procedures into two distinctive categories based upon the error criterion used in the formulation. His classification is intrinsically consistent with *Neuman*'s [1973]. Therefore the inverse solution methods in this literature survey are classified as that given by *Neuman* [1973] : (1) direct method (or equation error criterion) and (2) indirect method (output error criterion)

### 2.3.1 Equation Error Criterion

If the head variations and derivatives (usually estimated) are known over the entire flow region and if measurement and model structure errors are negligible, the original governing equations becomes a linear first-order partial differential equation of the hyperbolic type in terms of the unknown parameters. With the aid of boundary conditions and flow data, a direct solution for the unknown parameters may be possible. In practice, observation wells are sparsely distributed in the flow region and only a limited number of observation wells are available. Therefore missing data has to be estimated by interpolation (which contains errors in interpolation) in order to formulate the inverse problem by the equation error criterion. If the interpolated data along with observations (which also contains noise) are substituted into the governing equation, an error term results. The error is then minimised over the proper choice of parameters.

Among the available techniques of the equation error criterion, mention may be made of the energy dissipation method [*Nelson*, 1968]; linear programming [*Kleinecke*, 1971]; the use of flatness criterion [*Emsellem and de Marsily*, 1971]; the multiple objective decision process [*Neuman*, 1973]; the Galerkin method [*Frind and Pinder*, 1973]; the algebraic approach [*Sagar et al.*, 1975]; the inductive method [*Nutbrown*, 1975]; linear programming and quadratic programming [*Hefez et al.* , 1975]; minimisation of a quadratic objective function with penalty function [*Navarro*, 1977]; and the matrix inversion method with kriging [*Yeh et al.*, 1983].

### 2.3.2 Output Error Criterion

The criterion used in this approach is generally the minimisation of a *norm* of the difference between observed and calculated heads at specified location. The major advantage of this approach is that the formulation of the inverse problem is applicable to situations where the number of observations is limited, and it does not require differentiation of the measured data. A disadvantage of this approach is that minimisation is usually nonlinear and nonconvex. In general, optimisation starts with a set of initial estimates of the parameters and improves it in an iterative fashion until the system model response is sufficiently close to that of the observations.

Control-oriented techniques, stemming from the concept of quasilinearization of *Bellman and Kalaba* [1965], have been developed for aquifer parameter identification. Among the published works, mention may be made of the following: quasilinearization [*Yeh and Tauxe*, 1971; *DiStefano and Rath*, 1975]; minimax and linear programming *[Yeh and Becker*, 1973]; and the maximum principle [*Lin and Yeh*, 1974*; Yakowitz and Noren*, 1976]. *Vermuri and Karplus* [1969] formulated the inverse problem in terms of optimal control and solved it by the gradient procedure. *Chen et al.* [1974] also treated the problem in an

optimal control approach and solved it by both a steepest decent method and conjugate gradient method. Kalman filtering techniques have also been proposed in the literature for parameter identification [*McLaughlin*, 1975; *Wilson et al.*, 1978]. *Kitanidis and Vomvoris* [1983] used the technique of maximum likelihood estimation and kriging.

Mathematical programming techniques developed in the field of operations research have been utilised for solving the inverse problem of parameter identification in groundwater hydrology and in the field of petroleum engineering. Among the published reports, mention may be made of the following: gradient search procedures [*Jacquard and Jain*, 1965; *Thomas et al.*, 1972]; decomposition and multilevel optimisation [*Haimes et al.*, 1968]; linear programming [*Coats et al.*, 1970; *Slater and Durrer*, 1971; *Yeh*, 1975a,b]; quadratic programming [*Yeh*, 1975a,b; *Chang and Yeh*, 1976]; the Gauss-Newton Method [*Jahns*, 1966; *McLaughlin*, 1975]; the modified Gauss-Newton method [*Yoon and Yeh*, 1976; *Yeh and Yoon*, 1976; *Cooley*, 1977, 1982]; the Newton-Raphson method [*Newman and Yakowitz*, 1979] and the conjugate gradient method [*Neuman*, 1980].

## 2.4 Parameter Dimension and Parameterization

Parameters such as transmissivity, are continuous functions of the spatial variables. For identification purposes, a continuous function must be approximated by a finite dimensional form. The reduction of parameter dimensions is done by parameterization and the two techniques available in the literature are : (1) zonation method, and (2) interpolation method.

### 2.4.1 Zonation Method

In this approach, the flow region is divided into a number of subregions, or zones, and a constant parameter value is used to characterise each zone. The unknown transmissivity function, for example, is then represented by a number of functions which is equal to the number of zones. The dimension of parameterization is then represented by the number of zones times the number of parameters in the model under estimation. The zonation technique has been adopted by among others, *Coats et al.*, [1970], *Emsellem and de Marsily* [1971], *Yeh and Yoon* [1976], and *Cooley* [1977,1979].

### 2.4.2 Interpolation Method

If finite elements are used as the interpolation method, the flow region is divided into a number of elements connected to a number of nodes. Each node is associated with a local basis function. Then the unknown transmissivity, for instance, is approximated by a linear combination of the basis functions, where the parameter dimensions corresponds to the number of unknown nodal transmissivity values. Here the works by *DiStefano and Rath* [1975], *Yoon and Yeh* [1976], and *Yeh and Yoon* [1981] are worth mentioning. In the context of interpolation, other schemes such as spline [*Sagar et al.*, 1975; *Yakowitz and Noren*, 1976]; polynomial method [*Garay et al.*, 1976] and kriging [*Clifton and Neuman*, 1982], have been used to approximate the parameter distribution. The reduction of the number of unknown parameters by representing the parameters by a geostatistical structure as suggested by *Kitanidis and Vomvoris* [1983] is also classed under the method of interpolation.

However, one problem that still remains is how to determine the shape of zones in the zonation case or how to optimally determine the location of nodes in the interpolation

case. Most of the published work on this issue relies on trial-and-error approach or hydrological mapping.

## 2.5 Inverse Solution Techniques

A typical groundwater flow equation is used to illustrate some typical techniques that have been used to solve the inverse problem. Consider an unsteady flow in an inhomogeneous, isotropic and confined aquifer for which the governing equation can be represented by

$$\frac{\partial}{\partial x}\left(T\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(T\frac{\partial h}{\partial y}\right)=Q+S\frac{\partial h}{\partial t} \tag{2.1}$$

subject to the following initial and boundary conditions:

$$\begin{aligned} &h(x,y,0)=h_0(x,y), && x,y\in\Omega \\ &h(x,y,t)=h_1(x,y,t) && x,y\in\partial\Omega_1 \\ &T\frac{\partial h}{\partial n}=h_2(x,y,t) && x,y\in\partial\Omega_2 \end{aligned} \tag{2.2}$$

where:

| | |
|---|---|
| $h(x,y,t)$ | hydraulic head [$L$], |
| $T(x,y)$ | transmissivity [$L^2T^{-1}$], |
| $S$ | storage coefficient [$L^0$], |
| $Q(x,y)$ | volumetric rate of source-sink term per unit area [$LT^{-1}$], |
| $x,y$ | space variables [$L$], |
| $t$ | time [$T$], |

| | |
|---|---|
| $\Omega$ | flow region |
| $\partial\Omega$ | aquifer boundary ( $\partial\Omega_1 \cup \partial\Omega_2 = \partial\Omega$ ), |
| $\partial/\partial n$ | normal derivatives, and |
| $h_0, h_1, h_2$ | specified functions [$L$] |

For illustrational purposes it is assumed that the storage coefficient is known and the parameter chosen for identification is the transmissivity function, $T(x,y)$, which is assumed to be time invariant. In general a numerical scheme is required to obtain solutions of (2.1) subject to conditions (2.2), provided the parameter values are properly estimated. Various finite difference methods (FDM) or finite element methods (FEM) have been developed for numerical simulation studies. However, whether one chooses to formulate (2.1) with either the FDM or the FEM, the eventual system of algebraic equations that must be solved for the hydraulic heads, $h(x,y,t)$, is always of the form

$$CH = F \tag{2.3}$$

where:

| | |
|---|---|
| $C$ | coefficient matrix, a function of $T$, |
| $H$ | unknown hydraulic head vector containing values at all grid points, and |
| $F$ | column vector containing head values. |

In general, two methods are available in the literature for the inverse solution of $T$ given known values of heads in the simulation region : (1) generalised matrix method based upon the equation error criterion, and (2) Gauss-Newton minimisation based upon the output error criterion.

### 2.5.1 Generalised Matrix Methods

The generalised matrix methods is based upon the equation error criterion. When the equation error criterion is employed for parameter estimation, it requires an explicit formulation of the unknown parameters. Suppose head observations are available at each of the grid points and these observations are substituted into (2.3), then the system of equations to be solved can be written as

$$A_t T_g = b_t + \varepsilon_t \tag{2.4}$$

where:

$A_t$ coefficient matrix, a function of $h$,

$T_g$ unknown transmissivity tensor containing values at all grid points,

$\varepsilon_t$ resulting equation error, and

$b_t$ column vector.

In a more compact matrix form, (2.4) becomes

$$AT_g = b + \varepsilon \tag{2.5}$$

where:

$$A = \left[A_1{}^T, A_2{}^T, \ldots, A_N{}^T\right]^T$$

$$b = \left[b_1{}^T, b_2{}^T, \ldots, b_N{}^T\right]^T$$

$$\varepsilon = \left[\varepsilon_1{}^T, \varepsilon_2{}^T, \ldots, \varepsilon_N{}^T\right]^T$$

$T$ is a transpose operator when used as a superscript. When the FEM or FDM is used as the forward solution method, the resulting equation error, $\varepsilon$, will always be of the form of

(2.5). The advantage of this equation is that (2.5) is linear, and $T_g$ can be determined by minimising the equation error, $\varepsilon$. From (2.5), the least squares error (or residual sum of squares) can be expressed by

$$\varepsilon^T \varepsilon = \left(AT_g - b\right)^T \left(AT_g - b\right) \tag{2.6}$$

Minimising the least square error, the transmissivity vector can be obtained as

$$T_g = \left(A^T A\right)^{-1} A^T b \tag{2.7}$$

Solution (2.7) implicitly assumes homoscedasticity and lack of correlation among residuals. The solution is also highly dependent on the level of discretization used in the numerical solution of the governing equation. Another disadvantage is that the solution of (2.7) is generally unstable in the presence of noise.

### 2.5.1 Gauss-Newton Minimisation Methods

The Gauss-Newton method is based on the output error criterion. The objective is to determine *T(x,y)* from a limited number of observations of *h(x,y,t)* scattered in the field so that a certain criterion is optimised. If the classical least squared error is used to represent the output error, the objective function to be minimised is

$$\min J_{T(x,y)} = \left[h_D - h_D^*\right]^T \left[h_D - h_D^*\right] \tag{2.8}$$

where $h_D$ is the vector of calculated heads at observation wells, based upon some values of estimated parameters, and $h_D^*$ is the vector of observed heads. For identification purposes,

$T(x,y)$, can be parameterized by either the zonation or interpolation method mentioned earlier.

The Gauss-Newton algorithm has proven to be an effective algorithm for performing minimisation. The original and modified version of the algorithm has been used by many researchers in the past in solving the inverse problem, eg., *Jacquard and Jain* [1965]; *Jahns* [1966], *Thomas et al.*, [1972], *Gavalas et al.* [1976], *Yoon and Yeh* [1976], and *Cooley* [1977, 1982]. The popularity of the algorithm stems from the fact that it does not require the calculation of the of the Hessian matrix as required by the Newton Method and the rate of convergence is superior when compared to the classical gradient searching procedures. The algorithm is basically developed for unconstrained minimisation. However, constraints such as upper and lower limits are easily incorporated in the algorithm with minor modifications. The algorithm starts with a initial estimates of parameters and converges to a local optimum. If the objective function is convex, the local optimum would be the global optimum. However, due to the presence of noise in the observations, the inverse problem is usually nonconvex, and hence only a local optimum can be assured in the minimisation.

If $T$ is a vector that contains parameters $[T_1, T_2, \ldots, T_L]$, the algorithm generates the following sequence for an unconstrained minimisation problem :

$$\overline{T}^{k+1} = \overline{T}^{k} - \rho^{k} d^{k} \tag{2.9}$$

with

$$A^{k} d^{k} = g^{k} \tag{2.10}$$

where:

$$A^{k} = \left[J_D\left(\overline{T}^{k}\right)\right]^{T}\left[J_D\left(\overline{T}^{k}\right)\right],$$

$$g^{k} = \left[J_D\left(\overline{T}^{k}\right)\right]^{T}\left[h_D\left(\overline{T}^{k}\right) - h_D^{*}\right]$$

$J_D$ Jacobian matrix of heads with respect to $\overline{T}$ $[ML]$

$\rho^k$ step size [$L^0$],

$d^k$ Gauss-Newton direction vector [$L$],

$M$ number of observations, and

$L$ parameter dimension.

Occasionally the direction matrix [$J_D{}^T J_D$] may become ill-conditioned and correction must be made in order for the algorithm to continue. The elements of the Jacobian matrix are represented by the sensitivity coefficients,

$$J_D = \begin{bmatrix} \frac{\partial h_1}{\partial T_1} & \frac{\partial h_1}{\partial T_2} & \cdots & \frac{\partial h_1}{\partial T_L} \\ \frac{\partial h_2}{\partial T_1} & \frac{\partial h_2}{\partial T_2} & \cdots & \frac{\partial h_2}{\partial T_L} \\ \cdot & & & \\ \frac{\partial h_M}{\partial T_1} & \frac{\partial h_M}{\partial T_2} & \cdots & \frac{\partial h_M}{\partial T_L} \end{bmatrix} \tag{2.11}$$

where $M$ is the total number of observations, and $L$ is the total of parameters. The transpose of the Jacobian matrix , $J_D{}^T$ is obtained by switching respective row and column elements of the Jacobian matrix, $J_D$ to obtain

$$J_D{}^T = [J_D]^T = \begin{bmatrix} \frac{\partial h_1}{\partial T_1} & \frac{\partial h_2}{\partial T_1} & \cdots & \frac{\partial h_M}{\partial T_1} \\ \frac{\partial h_1}{\partial T_2} & \frac{\partial h_2}{\partial T_2} & \cdots & \frac{\partial h_M}{\partial T_2} \\ \cdot & & & \\ \frac{\partial h_1}{\partial T_L} & \frac{\partial h_2}{\partial T_L} & \cdots & \frac{\partial h_M}{\partial T_L} \end{bmatrix} \tag{2.12}$$

In solving the inverse problems, efficient methods are required for the calculation of the sensitivity matrix. In general three methods are available in the literature. These methods are presented in the next section.

## 2.6 Computation of Sensitivity Coefficients

Sensitivity coefficients, the partial derivatives of head with respect to each of the parameters under estimation, play an important role in the solution of the inverse problem. In the Gauss-Newton algorithm, elements of the Jacobian matrix are represented by the sensitivity coefficients, $\frac{\partial h_i}{\partial T_l}$, $i = 1,\ldots,M$, $l = 1,\ldots,L$. A literature survey indicates that three methods: (1) influence coefficient method, (2) sensitivity equation method, and (3) variation method have been used in the past for the calculation of sensitivity coefficients.

### 2.6.1 Influence Coefficient Method

The influence coefficient method [*Becker and Yeh,* 1972] uses the concept of parameter perturbation where the *lth* row of the $J_D{}^T$ is approximated by

$$\frac{\partial h_i}{\partial T_l} \approx \frac{h_i\left(\overline{T} + \Delta T_l e_l\right) - h_i\left(\overline{T}\right)}{\Delta T_l} \quad i = 1,\ldots,M, \quad l = 1,\ldots,L \tag{2.13}$$

where $\Delta T_l$ is the small increment of $T_l$, and $e_l$ is the *lth* unit vector. The values of $h\left(\overline{T}\right)$ and $h\left(\overline{T} + \Delta T_l e_l\right)$ are obtained by solving the governing equation (simulation), subject to the imposed initial and boundary conditions. The method requires perturbing each parameter one at a time. If there are $L$ parameters to be identified the governing equation

has to be solved $L$+1 times for each iteration in the nonlinear least square minimisation to numerically produce the sensitivity coefficients.

### 2.6.2 Sensitivity Equation Method

In this approach, a set of sensitivity equations are obtained by taking the partial derivatives with respect to each parameter in the governing equation and initial and boundary conditions. After taking the partial derivatives, the following set of sensitivity equations are obtained

$$\frac{\partial}{\partial x}\left[\frac{\partial\left(\frac{\partial h}{\partial T_l}\right)}{\partial x}\right]+\frac{\partial}{\partial y}\left[\frac{\partial\left(\frac{\partial h}{\partial T_l}\right)}{\partial y}\right]=S\frac{\partial\frac{\partial h}{\partial T_l}}{\partial t}+\left[-\frac{\partial}{\partial x}\left(\frac{\partial T}{\partial T_l}\frac{\partial h}{\partial x}\right)-\frac{\partial}{\partial y}\left(\frac{\partial T}{\partial T_l}\frac{\partial h}{\partial y}\right)\right] \qquad (2.14)$$

$$l=1,\ldots,L$$

The associated initial and boundary conditions are

$$\frac{\partial h(x,y,0)}{\partial T_l}=0 \quad l=1,\ldots,L$$

$$\frac{\partial h(x,y,t)}{\partial T_l}=0 \quad l=1,\ldots,L$$

$$T\frac{\partial\left(\frac{\partial h}{\partial T_l}\right)}{\partial n}=-\frac{\partial T}{\partial T_l}\frac{\partial h}{\partial n} \quad l=1,\ldots,L \qquad (2.15)$$

The number of simulations required to generate the sensitivity coefficients per iteration is $L$+$1$, which is the same as the influence coefficient method.

### 2.6.3 Variational Method

The variational method was first used for solving the inverse problem of parameter identification by *Jacquard and Jain* [1965] and then by *Carter et al.* [1974,1982] associated with the finite difference schemes. *Sun and Yeh* [1985] extended the method to the case of finite element schemes. Following *Carter et al.*, [1974], the sensitivity coefficients can be computed by the following equation:

$$\frac{\partial h^{(j)}}{\partial T_i^{(i)}} = \iint_{(\Omega_i)} \int_0 \nabla q'(x,y,t-\tau) \nabla h(x,y,\tau) d\tau dx dy \quad j = 1,2,..,N_0 \quad i = 1,2,..,N_n \tag{2.16}$$

where:

| | |
|---|---|
| $(\Omega_i)$ | exclusive subdomain of node *i*, |
| $\nabla$ | gradient vector, |
| $h(x,y,t)$ | solution of the governing equation, |
| $N_0$ | number of observation wells, |
| $N_n$ | total number of nodes used in the numerical solution, and |
| $q'(x,y,t)$ | time derivative of $q(x,y,t)$. |

Comparing the above three methods in the calculation of sensitivity coefficients, the variational method is advantageous if $L > N_0$, the case where the number of parameters to be identified is greater than the number of observations. On the other hand if $N_0 > L$, the influence coefficient and sensitivity methods are preferred. To avoid instability when the data contains noise, the number of parameters to be identified is usually less than the number of observation wells. *DiStefano and Rath* [1975] pointed out that in order to obtain a set of sensitivity coefficients with acceptable accuracy, much smaller time steps are required. The need for an efficient method for calculating the sensitivity coefficients in

solving the inverse problem has also been pointed out by *Dogru and Seinfeld* [1981], *McElwee* [1982], and *Skyes et al.*, [1985].

## 2.7 Uncertainty and Optimum Parameter Dimension

In field practice, the number of observations is limited and observations are corrupted with noise. Without controlling parameter dimension , instability often results [*Yakowitz and Duckstein*, 1980]. Instability in the inverse problem results in parameters becoming unreasonably small (sometimes negative) and/or large if parameters are not constrained. In the constrained minimisation, instability is characterised by the fact parameter values keep bouncing back and forth between the upper and lower bounds. By reducing the parameter dimensions, the instability can be reduced or eliminated. It has generally been understood that as the number of zones increases, the modelling error decreases while the parameter uncertainty increases.

*Emsellem and de Marsily* [1971] were the first to consider the problem of optimal zoning pattern. *Yeh and Yoon* [1976] suggested a systematic procedure based upon a statistical criterion for the determination of an optimal zoning pattern. *Shah et al.* [1978] showed the relationship between the optimal dimensions of parameterization and observation in a considerable depth. The need to limit the dimension of parameterization has been further studied by *Yoon and Yeh* [1976], *Yeh et al.* [1983], and *Kintanidis and Vomvoris* [1983]. These authors have shown that the dimension of parameterization is directly related to the quantity and quality of observation data. The error in parameter uncertainty can be represented by a norm of the covariance matrix of the estimated parameters [*Yoon and Yeh*, 1976; *Shah et al.*, 1978]. The covariance matrix of the estimated parameters is defined by the expression

$$Cov(T^{est}) = E\left\{\left(\overline{T} - T^{est}\right)\left(\overline{T} - T^{est}\right)^T\right\} \tag{2.17}$$

where:

| | |
|---|---|
| $T^{est}$ | estimated parameters, |
| $\overline{T}$ | true parameters, |
| $E$ | mathematical expectation, and |
| $T$ | transpose of a vector when used as a superscript. |

The covariance matrix of the estimated parameters also provides information regarding the reliability of each of the estimated parameters. A well established parameter is generally characterised by a small variance as compared to an insensitive parameter that is associated with large variance.

## 2.8 Bayesian Estimation

Bayesian methods that incorporate prior information have also been applied to parameter identification [eg., *Gavalas et al.*, 1976]. The geological information required for Bayesian estimation includes the mean and covariance of the parameters. These are given by

$$\begin{aligned} E\left\{\overline{T}\right\} &= T_{mean} \\ E\left\{\left(T_i - T_{mean}\right)\left(T_j - T_{mean}\right)\right\} &= r_{ij} \end{aligned} \tag{2.18}$$

The value of $T_{mean}$ is considered to be known and the prior information can be obtained from geological measurements in the field. *Gavalas et al.* [1976] have shown that Bayesian estimation reduces to a quadratic minimisation problem, provided the parameters and the measurement errors are normally distributed and the model is linear in the parameters. When these conditions are not satisfied, a rigorous application of Bayesian estimation is impractical.

### 2.8.1 Composite Objective Function

*Gavalas et al.* [1976] proposed the following practical approach (which is similar to the least squared minimisation) where the objective function is given by

$$J = \sum_{i=1}^{M} \frac{1}{\sigma_i^2}\left(h_i - h_i^*\right)^2 + \lambda\left(\overline{T} - T_{mean}\right)^T R^{-1}\left(\overline{T} - T_{mean}\right) \qquad (2.19)$$

where $\lambda$ is a weighting factor ($0 \le \lambda \le 1$) and $\sigma_i^2$, $i$ = 1, 2, ..., $M$ is the variance of the measured error which is considered known and $R$ is correlation matrix of the estimated parameters. The second term in the objective function is the Bayesian term which penalises the weighted deviation of the parameter from their mean values. *Shah et al.* [1978] have demonstrated that if reliable prior information is available, Bayesian estimation will lead to a smaller variance of the error of estimation.

### 2.8.2 Kalman Filtering

The technique of Kalman filtering was originally developed in the field of optimal control [*Kalman*, 1960]. It has been successfully applied in aerospace engineering for the problem of optimal estimation and control of vehicle trajectory. The application of Kalman filtering to parameter estimation in groundwater requires expressing the groundwater model in terms of a state-space formulation that consists of a vector state equation and a vector observation equation. For parameter estimation, the state vector is augmented to include the parameter vector as another state variable. If the errors in the state and observation equations have zero mean and are of Gaussian process with known covariance matrices , Kalman filtering can be applied for simultaneous, recursive state, and parameter estimation.

Since prior information is generally required in the application of Kalman filtering, it can be classified in the Bayesian estimation category. *Wilson et al.* [1978] used an extended Kalman filter for parameter estimation in groundwater. Their approach permits the utilisation of prior information about the parameters and information taken from input-output measurements to improve estimates of parameters as well as the system state.

## 2.9 Other Statistical Methods with Prior Information

*Neuman and Yakowitz* [1979] proposed a statistical approach to the inverse problem of parameter estimation. Their approach differs from the Bayesian estimation of *Gavalas et al.* [1976] in that prior information may include actual values of transmissivity determined from pumping tests or other measurements at specific locations in the aquifer, or it may be based on statistical information about the spatial variability in other aquifers consisting of

similar materials [*Neuman and Yakowitz*, 1979]. The composite objective function proposed by Yakowitz and Newman is similar to that of *Gavalas et al.* [1976] and can be expressed as

$$J = \left[h^* - f(\overline{T})\right]^T V_h^{-1}\left[h^* - f(\overline{T})\right] + \lambda\left(T^* - \overline{T}\right)^T V_T^{-1}\left(T^* - \overline{T}\right) \tag{2.20}$$

where:

$T^*$ prior estimate of $\overline{T}$,

$V_T$ known symmetric positive definite matrix,

$V_h$ known matrix, symmetric and positive definite,

$\lambda$ unknown positive parameter,

$f(\overline{T})$ model solution, and

$h^*$ observed head.

Neuman and Yakowitz proposed two methods called cross-validation and comparative residual analysis, to select the optimum value of $\lambda$. *Neuman* [1980] developed an efficient conjugate algorithm for performing the minimisation of (2.20). He extended the variational method developed by *Chevant* [1975] for calculating the gradient with respect to the parameter in the case of the generalised nonlinear least square.

The composite objective function presented by *Abufirassi and Marino* [1984b] is again conceptually similar to *Gavalas et al.* [1976]. They used kriging to estimate the missing values of head and the value of the error covariance matrix, while cokriging [*Abufirassi and Marino*, 1984a] was used to estimate $T^*$ and the associated error covariance matrix. Cokriging [*Journel and Huijbregts*, 1978], an extension of kriging to

two or more variables, can be used to improve the accuracy of estimation of a variable that is not sufficiently sampled by considering its spatial correlation with other variables that are better sampled.

*Cooley* [1982] proposed a method to incorporate prior information on the parameters into the nonlinear regression model he developed [1977]. The primary purpose of Cooley's work was the incorporation of prior information of unknown reliability. A secondary purpose of Cooley's work was to incorporate Theil's [1963] model into Cooley's [1977] nonlinear regression model where at least some prior information of known reliability is available. The approach is non Bayesian in the sense that no prior distribution of the parameter is assumed. The approach also differs from the method proposed by Neuman and *Yakowitz* [1979] and *Neuman* [1980] primarily in two ways : (1) the prior information in Cooley's work is considered to consist of a general nonlinear combination of several types of parameters as opposed to the direct estimate of a single type of parameter and (2) the way in which the covariance structure of the model is determined.

*Kitanidis and Vomvoris* [1983] proposed a geostatistical approach for solving the inverse problem. Their method consists of two main steps : (1) the structure of the parameter field is identified and (2) kriging is applied to provide minimum variance and unbiased point estimates of hydrogeological parameters using all available information. In their approach, it is assumed that several point measurements of head and transmissivity are available. In effect, parameterization is achieved by representing the hydrogeological parameters as a random field which can be characterised by the variogram and trend with a small number of parameters. *Hoeksema and Kitanidis* [1984] have applied the geostatistical approach to the case of a two-dimensional steady state flow. A finite difference numerical model of groundwater was used to relate the head and transmissivity variable and cokriging was used to estimate the unknown transmissivity field. *Dagan* [1985] has also considered the geostatistical technique using an analytical and Gaussian conditional mean in place of Kriging. Hoeksema and Kitanidis made a comparative study of Dagan's approach and

Kriging estimation. In using the geostatistical approach, it is implicitly assumed that transmissivity has a low variability.

## 2.10 Summary of the Inverse Problem Survey

From the foregoing, it is clear that parameter estimation in groundwater modelling has been completely dominated by the gradient-based techniques; it is also clear that considerable attention has been given to parameter estimation of flow models. In essence, parameter identification of solute transport models has received little attention. In the context of performance a considerable success of the gradient-based techniques has been achieved. However, the problem of parameter instability and ill-conditioning of the sensitivity matrix (in some problems) has not yet been resolved. All the three techniques available for the computation of the sensitivity matrix have their advantages and disadvantages. For example, it is known that if the number of parameters under estimation is greater than the number of observation points, the influence coefficient and the sensitivity equation methods may not work properly while the variational method is bound to produce unreliable results when the number of observations points is greater than the parameters under estimation. The problem with parameter uncertainty and optimum parameter dimensions also limits the application of the gradient-based methods to relatively simplified cases of groundwater parameter estimation since one has to reduce the dimensionality of the problem in order to avoid instability .

## 2.11 The Shuffled Complex Evolution

A recent study by *Duan et al.* [1992] on a six-parameter model using synthetic data to identify the nature of difficulties usually encountered in the calibration of conceptual rainfall-runoff (CRR) models uncovered five major problems that complicate the solution process of model calibration (or the inverse problem) : (1) there may be several major regions of attraction into which the search strategy may converge, (2) each major region of attraction may contain numerous local minima which may occur both close to and at various distances from the best solution, (3) the objective function surface in the multiparameter space may not be smooth and continuous, and the derivatives may be discontinuous and vary in an unpredictable manner through the parameter space, (4) the parameters may exhibit varying degrees of sensitivity and a great deal of interaction and compensation, and much of the interaction can be highly nonlinear, and (5) the response surface near the true solution is often nonlinear. An optimisation algorithm that deals with the problems enumerated above must possess the following qualities : (1) global convergence in the presence of multiple regions of attraction, (2) ability to avoid being trapped by 'pits' and 'bumps' over the objective function surface, (3) robustness in the presence of differing parameter interdependencies, (4) nonreliance on the availability of an explicit expression for the objective function or the derivatives, and (5) capability of handling high parameter dimensionality. All these qualities are possessed by the Shuffled Complex Evolution (SCE) methodology. The SCE methodology was developed by *Duan et al.* [1992,1993] purposely for the calibration of difficult and complex CRR models.

The SCE is based on the synthesis of four concepts that has been proved to be successful in the past : (i) combination of deterministic and probabilistic approaches, (ii) systematic evolution of a complex of points spanning the parameter space, (iii) competitive evolution, and (iv) complex shuffling. The synthesis of these four concepts makes the SCE method not only effective and robust but also flexible and efficient. The use of deterministic

strategies permit the SCE algorithm to make effective use of the response surface information to guide the search. Robustness and flexibility are taken care of through the inclusion of random elements. Concentrating a search in the most promising region of the search space is guided by the implicit clustering strategy. The use of systematic complex evolution strategy helps to ensure a relative robust search that is guided by the structure of the objective function. The present literature survey has indicated that no attempt has been made to extend the SCE methodology to parameter estimation (or the inverse problem) in the context of groundwater modelling. Therefore in this aspect of the current research work, an attempt is made to achieve this objective. The SCE methodology is described in detail in section 5.3.

## 2.12 Groundwater Resources Management

In the past two decades, the field of groundwater hydrology has turned toward numerical simulation models to help evaluate groundwater resources. The application of the finite difference and finite element methods to groundwater equations have permitted complex, real world systems to be modelled. Numerical simulation models have enabled hydrogeologists to develop a better understanding of the functioning of regional aquifers and to test hypotheses regarding the behaviour of particular facets of groundwater systems. Additionally, simulation models are often utilised to explore groundwater quality and quantity management alternatives. In such cases a model is executed repeatedly under various design scenarios in an attempt to achieve a particular objective, such as isolating the plume of contaminated groundwater, preventing saltwater intrusion, dewatering an excavated area, or obtaining a sustainable water supply. This aspect of the literature review concerns the joint use of simulation models and optimisation methods designed for

management decision purposes. Only those management models which simulate groundwater hydraulics or groundwater solute behaviour by solving the partial differential equation are mentioned.

## 2.13 Groundwater Quantity Management

Studies which combine aquifer simulation with management models in the context of groundwater quantity may be grouped into two categories : (1) groundwater hydraulic management and (2) groundwater policy evaluation and allocation. In the first category, models are aimed at managing groundwater stresses such as pumping and recharge, wherein the stresses and hydraulic heads are treated directly as management model decision variables. The second category involves models that can be used to inspect complex economic interactions such as the influence of institution upon the behaviour of an agricultural economy or complex groundwater-surface water allocation problems. In both categories, the models employ the optimisation techniques of linear or quadratic programming, which attempt to optimise an objective such as minimisation of costs or maximisation of well production; and are subject to a set of linear algebraic constraints which limit or specify the values of the decision variables such as local drawdowns, hydraulic gradients, and pumping rates.

In both categories the simulation model component of the management models is based upon the equation of groundwater flow in saturated porous media [*Cooper*, 1966; *Pinder and Bredehoeft*, 1968; *Remsen et al.*, 1971]. For a nonsteady two-dimensional, heterogeneous , and anisotropic case, the equation is expressed as

$$\frac{\partial}{\partial x_i}\left(T_{ij}\frac{\partial H}{\partial x_j}\right) = S\frac{\partial H}{\partial t} + W \qquad i,j = 1,2 \tag{2.21}$$

where:

$T_{ij}$ transmissivity tensor [ $L^2T^{-1}$ ],

$H$ hydraulic head [$L$],

$W$ volumetric flux per unit area [ $LT^{-1}$ ],

$S$ storage coefficient [ $L^0$ ],

$x_i, x_j$ cartesian coordinates [$L$], and

$t$ time [$T$]

### 2.13.1 Groundwater Hydraulic Management Models

Groundwater hydraulic management models incorporate the simulation model of a particular groundwater system as constraints in the management model. Management decisions as well as simulation of groundwater behaviour are accomplished simultaneously. Two techniques namely : (1) embedding method and (2) the response matrix approach have been derived to accomplish this. In the embedding method, finite difference or finite element approximations of the governing groundwater flow equations are treated as part of the constraint set of a linear programming model. Decision variables are hydraulic heads at each node as well as local stresses such as pumping rates and boundary conditions. In the response matrix approach, an external groundwater simulation model is used to develop unit responses. Each unit response describe the influence of a pulse stimulus upon hydraulic heads at points of interest throughout the system. An assemblage of the unit responses, and a response matrix are included in the management model. The decision variable in a linear, mixed integer, or quadratic program include the local stresses such as pumping or injection rates. It may include hydraulic heads at the discretion of the modeller.

### 2.13.1.1 Embedding Method

The embedding method for the hydraulic management of aquifers uses linear programming formulations that incorporate numerical approximations of the groundwater equations as constraints. This technique was initially presented by *Aguado and Remsen* [1974] for groundwater hydraulic management where they demonstrated with one- and two-dimensional examples that the physical behaviour of the groundwater system could be included as an integral part of an optimisation model. They used finite difference approximations in both steady and transient problems for confined and unconfined aquifers. In all examples, physical objective functions maximised hydraulic heads at specified locations and constraints were placed upon heads, gradients, and pumping rates. For the confined case, the governing equation was linear, and the resulting finite difference approximations were treated as linear constraints. For the unconfined case the steady state equation was treated as linear with respect to the square of the hydraulic heads.

*Aguado and Remsen* [1974] presented a real world example for determining the optimal steady state pumping scheme to maintain groundwater levels below specified elevations for a dry rock excavation site. The solution to the dewatering problem indicated that the minimum total pumping could be accomplished by developing the maximum number of wells as close to the excavation as the finite difference grid will allow. In a later study [*Aguado and Remsen*, 1980], set up costs were included by reformulating the problem as a *fixed charge problem* where costs due to pumping plus fixed costs due to well installations were considered. When penalties were assessed for well installation and development, the solution lost its strong dependence on the finite difference grid.

*Alley et al.* [1976] presented a report on aquifer management under transient conditions using the embedding technique and treating the finite difference form of the confined aquifer as constraints in a linear problem. Their illustrative example sought to

maximise hydraulic heads while obtaining specified flow rates from wells within the system. The transient behaviour was treated by creating successive management models; one for each time step. The optimal solution for one time step was treated as initial conditions for next management model. In comparison, the transient management approach of *Aguado and Remsen* [1974] was to lump all time step models as constraints in one linear program. This approach enabled short-range aquifer management goals to be included in the context of long range management goals but could result in a very large matrix. The method of *Alley et al.* [1976] required optimisation of several smaller single time step models. The deficiency in this latter approach is that management decision on the short range term may contradict long range management requirements.

*Schwarz* [1976] suggested incorporating as linear programming constraints a series of mass balances among cells which comprise an aquifer. *Schwarz* [1976] noted that the transformation model represents properties of the aquifer by water level transformation equations for discrete cells. The transformation equation approach of Schwarz is essentially the same as the embedding approach in that a model which was discretized over space and time was included as linear programming constraints. The difference is that the transformation model depended on a multicell aquifer model, while the embedding models employed finite differences or finite elements.

The embedding technique has been demonstrated for cases involving hydraulic gradients control using injection and pumping wells. *Molz and Bell* [1977] applied the technique to a hypothetical case involving the steady state control of hydraulic gradients to insure the stationarity of a fluid stored in an aquifer. Their linear program contained constraints which consisted of the confined groundwater flow equation in finite difference form. They constrained gradients to fixed values in the region of their five-point well scheme. The objective function was to minimise the total of pumping plus injection. Solutions were achieved for their 81 node model with minimal computational requirement. *Remsen and Gorelick* [1980] demonstrated the embedding approach to control hydraulic

gradients in order to contain a plume of contaminated groundwater. This was done in the context of other regional management goals, including the dewatering of two excavation areas and obtaining water for export from the system. The objective was to minimise pumping. The solution selected those nodal locations where either pumping or injection wells should be located. Furthermore, it determined the optimal pumping rates, and gave the resulting steady state hydraulic head solution for 99 active nodes.

Although management models have been solved successfully, it is noted that no large-scale application of the embedding approach has ever been reported. It seems that numerical difficulties are likely to arise for large-scale problems if linear programming solution techniques are utilised. Commercial codes try to maintain the sparsity of the matrix upon which linear programming operations are performed. Numerical difficulties usually occur with lower-upper basis factorisation when banded matrices are involved. The discretization of groundwater flow equations using finite differences or finite elements yields a banded matrix. *Elango and Rouve* [1980] have experimented with the finite element and linear programming method and hypothesised that problems may arise when a large number of equality constraints are considered.

#### 2.13.1.2 Response Matrix Approach

The second technique in groundwater hydraulic management is the response matrix approach. Incorporation of a response matrix into a linear program was initially proposed in the petroleum engineering literature by *Lee and Aronofsky* [1958]. They developed a linear programming management model which sought to maximise profit from oil production. A response matrix was used to linearly convert pumping stresses into pressure changes in the petroleum reservoir. The pressure response coefficients were developed using an analytic solution of the flow equation. Constraints ensured that reservoir pressures were maintained

above one atmosphere, limited total production to the reservoir capacity, and guaranteed that oil purchased from an outside source did not exceed the pipeline capacity. Their solution gave optimal production rates for each of five potential sources during four time periods of two years each. *Aronofsky and Williams* [1962] extended this work to the scheduling of drilling operations.

*Wattenbarger* [1970] presented a method to maximise total withdraws from a gas reservoir. He noted that for any number of wells in the reservoir, it is necessary to know only each well's own drawdown curve and interference curves for each pair of wells in a reservoir. The pressure behaviour at each well can be calculated through superposition for any rate schedule. He formulated his problem as a linear programming management model wherein his objective was to maximise well production. Constraints based upon the matrix response served to maintain pressures above critical values at each well. Additional constraints established the maximum reservoir withdrawal rate by forcing the total production rate not to exceed projected gas demand. Wattenbarger made one final important comment. *A constraint matrix which includes the response matrix relations will generally be extremely dense for linear programming problems. If off diagonal entries of the response matrix are extremely small, they may be neglected and set to zero thereby decreasing the matrix density. This technique can make large-scale problems much more manageable.*

The response matrix soon became established in the groundwater literature. *Deninger* [1970] considered maximisation of water production from a well field where he proposed that drawdown responses be calculated using the nonequilibrium formula of *Theis* [1935]. The linear programming formulation sought to maximise total well discharge. Constraints were written to limit drawdowns and account for pump and well facility limitations. Of greater significance, Deninger also presented a management formulation to minimise the cost of water production. Both discharge rates and lifts were unknown prior to

solution. The use of quadratic programming was suggested to solve this problem but no solutions were presented.

*Maddock* [1972a] solved the nonlinear problem of minimising pumping costs. A constraint set which he called *algebraic technological function* was developed as a response matrix. The response coefficients showed drawdown changes induced by pumping at each well. He used a quadratic objective function that minimised the present value of pumping costs. In an example, he considered a complex heterogeneous groundwater system in which discharge from three wells was scheduled for 10 seasons. Constraints guaranteed meeting semiannual water targets and set upper limits on the pumping capacity of each well. A standard quadratic package [*Karash*, 1962] was used to solve the problem. *Maddock* [1974b] developed a nonlinear technological function for the unconfined aquifer case in which saturated thickness varies with drawdown. The solution of the nonlinear partial differential equation was given by an infinite series of solutions to linear partial differential equations. Drawdown was treated as a finite sum of a power series. With this technique, a quadratic program was formulated in which all the nonlinearities appeared in the objective function with constraints remaining linear.

Mixed integer programming has been used in conjunction with a response matrix to determine the optimum locations of wells. *Rosenwald* [1972] and *Rosenwald and Green* [1974] identified the best location for a specified number of wells so that the production demand curve is met as closely as possible. An external finite difference model was used to generate a transient response matrix which described pressure changes caused by pumping. This response matrix was used to develop constraints identical in form to those of *Wattenbarger* [1970]. However, integer constraints were added which specified the number of wells that were permitted to enter the solution. The management model maximised production within the demand constraints by selecting the best wells among the potential well sites. Optimal well selection was also the subject of *Maddock* [1972b], who developed a mixed integer quadratic programming model that minimised pumping costs plus

fixed costs for well and pipeline construction. The quadratic portion of the objective was made separable by a transformation that enabled solution by a combination of mixed integer and separable programming. Their study illustrated the sensitivity and error analysis to evaluate the effects on planning activities of uncertainty in economic and hydrologic factors.

*Rosenwald and Green* [1974] described a gas reservoir management case. The governing equation was nonlinear, and linear superposition (required in the response matrix approach) did not yield an adequate approximation. Attempts were made to develop iteration procedures which utilised the information from the linear programming management model to improve the solution. In the first method adjustments were made to the allowable drawdown. A revised linear program was executed, but validation with the nonlinear simulation model indicated that the revised permissible drawdowns were overcorrected. Increased pressure drop limits were used and a new management model executed. Solution verification indicated a better agreement, but some significant errors remained. *Rosenwald and Green* [1974] mentioned that one should be able to repeat the routine until closer agreement is obtained. The second iterative method used the results of the linear program to adjust the response matrix. The unit pumping rates used to generate the response matrix were revised and a new response matrix developed. Again, the updated linear programming management model results did not satisfy the nonlinear flow equation but did improve the solution.

Variations of the response matrix approach have been applied to the management of aquifer-stream systems. *Taylor* [1970] demonstrated with a very simple small problem how the conjunctive use of groundwater and surface water along the Arkansas river in Colorado could be managed using linear programming. A set of approximate response curves was developed which showed the average effect of aquifer stresses upon streamflow. The response curves were averaged over large cells which were roughly parallel to the river and extended along the entire stream reach. The objective was to minimise stream depletion

during two summer months. Constraints limited pumping in each cell, and specified the demand during each month from each cell.

*Morel-Seytoux* [1975 a,b] presented various linear programming formulations and solutions involving conjunctive surface-groundwater management. The response coefficient generator of *Morel-Seytoux and Daly* [1975] was used to develop response matrix constraints that predicted the reduction in return flow along a river reach due to pumping. Models were used to explore four management strategies. The first was to maximise total pumping during a growing season subject to a restriction that flow to the stream could not fall below a specified rate. A second model added a constraint that pumping during all weeks must be equal. A third model sought to minimise the need for water storage to meet demand with available supplies. Finally, a stochastic storage strategy used sequential solution which minimised the need for storage. Weekly updates of actual rather than expected river flow were used to calculate conditional expected flow for the remaining weeks. *Illangasekare and Morel-Seytoux* [1982] have linked response coefficient approaches for an aquifer and for a stream using a linear stream-aquifer interaction relationship. They concluded that the resulting stream-aquifer simulation model could be incorporated into a mathematical optimisation problem.

Applications of the response matrix approach to groundwater hydraulic management involving a large number of decision variables for regional aquifers have been demonstrated. *Larson et al.* [1977] constructed a management model to determine the safe yield of a groundwater system near Carmel, Indiana (referred to as the Carmel aquifer). Their management model maximised the steady state pumping rate by selecting from 199 potential well sites. Restrictions placed a lower limit on the pumping rate at each active well site and limited the number of permissible active wells. These restrictions led to a series of integer variables which specified whether a well exits at a particular well site. Other constraints forced pumping rates below design capacity and limited drawdown to one half the initial saturated thickness. The Carmel aquifer is unconfined and therefore was described by the

nonlinear Boussinesq equation. To linearize the system, steady state drawdowns for a confined aquifer were simulated and adjusted for unconfined conditions. The linear response matrix was created using the U.S. Geological Survey aquifer simulation model of *Trescott et al.* [1976]. Aquifer parameters calibrated by *Gillies* [1976] for the Carmel aquifer were used. In the solution, 26 well sites were selected and the distribution of pumping rates was determined. Drawdowns predicted at the well sites using a nonlinear simulation model compared favourably well with the results using the linearized and adjusted drawdowns. It was concluded that the linearization did not seriously affect the results.

*Willis* [1983] applied the response matrix approach to the agricultural Yun Lin basin, Taiwan. The linear programming problem was to determine the optimal pumping scheme for three consecutive periods in order to meet agricultural water demands. The objectives were to maximise the sum of the hydraulic heads and minimise the total water deficit. Constraints were placed on local groundwater demands, hydraulic heads, and well capacity. Of key interest was the use of quasilinearization to solve the equation describing transient unconfined flow. This yielded a linear approximation which required iteration to achieve a solution to the original Boussinesq equation. The iterative procedure used the head distribution from one linear programming solution to update the linearized response constraints for the next solution. The simulation model used a finite element network containing 101 nodes.

The response matrix approach has been applied to groundwater hydraulic management in the Pawnee Valley of south-central Kansas by *Heidari* [1982]. A groundwater model for the area was developed in prior studies by *Sophocleous* [1980] and the aquifer parameters were used in conjunction with the computer program of *Maddock* [1969] to generate the response matrix. As an approximation, the unconfined system was treated as a confined aquifer and drawdowns were corrected using *Jacob* [1944]. The response matrix was utilised in a linear program which maximised pumping rates over time. The total pumping during each time period was forced to meet demands and each pumping

rate was limited by water rights. Drawdown at any time was constrained to a fraction of the total saturated thickness. Different solutions were obtained under maximum drawdown fractions which ranged from 0.1 to 0.25. To reduce the number of decision variables, wells were clustered into 61 well fields. Models were run for a 5-year planning horizon and a 10-year planning horizon. In each case, the time horizon was broken down into five equal management time units of 1 and 2 years, respectively. By considering various sets of constraints in several model runs, *Heidari* [1982] was able to demonstrate that the response matrix is applicable to real world systems and is a valuable tool for evaluating groundwater management systems.

#### 2.13.1.3 Comparison of Hydraulic Management Methods

In the embedding approach, the discretized flow equations are included in the linear programming as constraints and a complete simulation model is solved as part of the management model. Hydraulic heads throughout the entire spatial domain and at each time step are treated as decision variables. The embedded simulation model yields a great deal of information regarding the aquifer behaviour. However, it will rarely occur that management involves all the hydraulic heads over space and time. Therefore, many of the decision variables and constraints will be unnecessarily contained in the linear programming model. For computational economy and avoidance of numerical difficulties, application of the embedding approach is limited to small steady state problems.

In the response matrix approach, solutions of the flow equations serve as linear programming constraints. This approach yields incomplete information regarding system functioning but is generally a more economical method. Development of the response matrix requires the solution of one external simulation model for each potentially managed

well or other excitation, such as local boundary condition. This may require a large initial expenditure of computational effort. However, the resulting response matrix is a more efficient, condensed simulation tool. Constraints are included only for specified locations and time. Unnecessary constraints or decision variables are not incorporated into the linear management model. Therefore, the response matrix approach can handle large transient systems in an efficient manner.

### 2.13.2 Groundwater Policy Evaluation and Allocation

Groundwater policy evaluation and allocation models are valuable for complex problems where hydraulic management is not the sole concern of the water planner. These models inspect water allocation problems involving economic management objectives. Such models have been applied to large-scale transient problems which study behaviour of an agricultural economy in response to institutional policies and to optimisation of conjunctive water use. Three types of models are available in the literature for groundwater policy evaluation and allocation problems : (1) hydraulic-economic response models, (2) linked simulation-optimisation models, and (3) hierarchical models. Hydraulic-economic response models are a direct extension of the response matrix approach to problems in which agricultural and/or surface allocation economics play a role. Linked simulation-optimisation models use results of an external aquifer simulation model as input to a series of subarea economic optimisation models. Information and results from each planning period are utilised for management during the next period. Because the simulation and economic management models are separate, complex social, political, and economic influence can be considered. Hierarchical models use subarea decomposition and a response matrix approach . Large and complex systems can be treated as a series of independent subsystems, and multiple objectives can be considered.

### 2.13.2.1 Hydraulic-Economic Response Models

The hydraulic response matrix has been extended to include agricultural-economic or surface water allocation management components. Each of these models is formulated as a single optimisation problem in which hydraulic and other controllable activities are considered. The first such combination of groundwater and economic management models was presented by *Maddock* [1974a]. A conjunctive stream-aquifer simulation model using finite differences was used to develop an algebraic technological function (response matrix). The planning model was developed for a hypothetical water management agency with the objective of minimising discounted expected value of water costs supplied by the stream aquifer system. Constraints included expected water demand, downstream water rights, water spreading for aquifer recharge, and stream-aquifer water transfers. Within the context of a quadratic programming problem, water demand was considered a stochastic process. A single planning model solution provided operating rules for groundwater withdrawals, stream diversions, water spreading, and return flow to the stream. Sensitivity of the model to variation in parameters, such as demand variance, was demonstrated.

*Maddock and Haimes* [1975] used the response matrix approach along with agricultural-economic considerations to study a tax-quota system for groundwater management to a hypothetical farming region. The scheme employed a quota in which each user was assigned an annual draft (resulting from the optimisation model) and a tax which would be assessed if this draft limit was exceeded. Farmers using less than a quota could be entitled to a rebate. A quadratic programming problem was formulated which sought to maximise combined net revenues on the farms and thereby determine pumping quotas. Linear constraints restricted drawdown and pumping rates using a hydraulic response

matrix. Additional linear constraints limited the acreage planted and guaranteed that irrigation water requirements were met. Response coefficients were developed and the optimisation model was solved for a 5-year planning horizon. The optimal solution gave the pumping quotas for each well in the system.

Economic management of an aquifer-stream system was the topic of *Morel-Seytoux et al.* [1980]. In an approach similar to *Maddock* [1974a], they demonstrated a link between an economic model and a hydrologic model in one quadratic programming formulation. In a hypothetical system, water for irrigation was supplied from groundwater and a river diversion. The objective of the model was to minimise the total cost of water. Constraints were placed upon water availability, water rights and land availability for each crop. Optimal crop yield as well as crop prices were known, and each crop yield was assumed to vary with the degree of irrigation. Pumping costs were related to groundwater drawdown. The model consisted of a quadratic objective function relating to water costs and a series of linear constraints. No solutions were presented; however, the authors noted that the solution could be achieved using existing techniques.

#### 2.13.2.2 Linked Simulation-Optimisation Models

Linked simulation-optimisation models were developed to study the impact of institutional changes upon groundwater use. The study of *Bredehoeft and Young* [1970] explored the effect of two policy instruments (a tax and quota) upon groundwater basin management. A complex hypothetical basin was considered for the temporal allocation of groundwater to agricultural users. The management objective was to maximise the net agricultural economic yield of the basin. An economic management model was formulated as a series of linear programming problems where crop acreage and the annual quantity of

water pumped were decision variables. One such model was formulated for each agricultural subarea, and separate models were solved for each 5-year management interval. An external numerical surface model provided input to the linear program as estimated annual cost of pumped water for each subarea. The finite difference model simulated transient unconfined flow for the regional aquifer. A sequential computational link was developed between the economic models and the groundwater simulation model. Preliminary subwater demands were computed using the linear program. Then calculations and checks were made regarding the profitability of reinvestment in wells, well life limits, and economic failure for each subarea. Pumping requirements were adjusted and the aquifer simulation rerun. The resulting hydraulic heads were used to compute estimated future pumping costs for the next 5-year interval in the economic linear programming models. The procedure was repeated for the next 50-year time horizon.

The linked model approach was further extended to the management of groundwater and surface water systems by *Young and Bredehoeft* [1972]. They studied an 80-km reach of the South Platte river in Colorado in which all groundwater ultimately came from the river. Their study considered an institutional framework which would tend to minimise the impact upon river flow of groundwater pumping for irrigation through examination of the policy implications of a basin authority for partial centralisation of control, allowed for the development of new water supplies. In this context, a model was developed which linked economic management with numerical simulation. As in their former studies, numerous linear programming models and periodic groundwater simulation models were executed. The goal of the basin authority was assumed to be maximisation of the average annual economic yield. A linear program was developed which maximised net revenues at the beginning of the simulation season. Constraints considered water acquisition, and irrigable land limitations. A sequence of computations then determined irrigation return flow, flow diversions, and crop acreages. Monthly subarea operating models were formulated as linear programs in which surface water use and groundwater use

were decision variables. The constraints related to irrigation requirements and local net revenues were maximised. After each subarea operating model was solved, an aquifer was executed for nongrowing seasons. The planning model was then run for the next irrigation season and the process repeated for a 10-year time horizon.

*Bredehoeft and Young* [1983] updated their 1972 model by considering the influence of certain surface water supplies. Their study was again patterned a reach of the South Platte River in Colorado , and the linked model approach was employed. In addition to maximising net revenue, they argued that farmers countered variance in income caused by short water supplies. Farming economics in the study area were such that reliance upon uncertain surface water supplies was unwise. Increasing well capacity so that all acreage could be irrigated by wells significantly reduced the variance of income. As in this study, the management modelling approach illustrates quantitatively that the development of the groundwater systems may be motivated by the desire to insure against periodic short water supplies. The study provided a more comprehensive framework to evaluate management institutions.

The linked simulation-optimisation approach was used by *Daubert and Young* [1982] to evaluate the influence of two groundwater management schemes along the lower South Platte River in Colorado. Their model was similar to that of *Young and Bredehoeft* [1972] but used the aquifer-stream response model of *Morel-Seytoux* [1975b] and contained a legal submodel which distributed surface water rights and groundwater with respect to assumed management policies. The management model was first concerned with a groundwater policy that effectively prohibited groundwater use during drought periods. The second policy regarded groundwater as a common property and limited pumping only by the well capacity. Results showed that while unrestricted groundwater use resulted in enhanced net income from irrigated farming, it imposed large external costs on surface water users who must cope with declining flows.

### 2.13.2.3 Hierarchical Models

The hierarchical approach was developed to model and optimise large scale water resource systems. The general approach has been described by *Haimes* [1977]. *Yu and Haimes* [1974] first employed this approach to optimise a complex regional groundwater allocation problem. They reasoned that a decomposition and multilevel approach breaks down a complicated regional resource management problem into smaller local level problems, each of which is optimised before attempting to optimise the overall regional problem. The process is iterative and requires coordination and feedback from the solution of the higher-level (overall) problem to local level optimisation.

They were concerned with planning to improve the allocative efficiency of the regional water resources, particularly groundwater. The regional problem was decomposed into subproblems, one for each subregion. Each subregion was formulated as a nonlinear mathematical programming problem which minimised net water supply costs, which were considered to be functions of water importation, pumping, and water levels. The aquifer model was a two-dimensional asymmetric polygonal finite difference system [*MacNeal*, 1953]. Subregional model solutions were fed to a second level representing coordination by a regional authority. The authority dealt with assuring consistent water levels across the individual polygonal regions, determined tax rates, and determined the optimal artificial recharge operation rate to minimise regional water supply costs. The interaction between the regional authority and subregions was accomplished using an iterative decision-making process. By structuring the model in this manner, decentralised decisions were tied together to solve a complex regional groundwater allocation problem by imposing a regional pumping tax to provide revenue for artificial recharge.

A multilevel management model for a complex groundwater-surface water system was presented by *Haimes and Dreizen* [1977]. It uses both the response matrix approach and a multilevel structure to optimise a complex, conjunctive system. Their strategy was to solve a series of optimisation models which employed response matrices. In the first stage, optimisation models were executed which maximised each water users net benefit. The problems were formulated as quadratic models in which decision variables were local pumping quantities, artificial recharge activity, and surface water use. Constraints specified water requirements, lift and pumping limitations for each well, recharge facility capacity, and surface water allocation. Response matrices were developed with the aquifer simulation program of *Maddock* [1969]. In their study, individual subarea models were solved using the multicell simulation technique by *Dreizen and Haimes* [1977].

The second stage of the multilevel optimisation scheme determined drawdowns throughout the system and flows induced from the river into the aquifer. This process was accomplished by summing the influences resulting from the solutions obtained for each area from the first stage in the optimisation. Net streamflow to the reservoir was calculated, reservoir overflow was checked, and reservoir operation costs were determined. These factors were then entered into an optimal surface water allocation program in which the reservoir capacity and periodic allocation limits served as constraints. A sample solution was presented over a 6-year planning horizon. The optimal solution indicated a well-pumping plan, recharge plan, and surface water use plan.

A hierarchical model has been developed by researchers at the World Bank to study groundwater and surface water policies for the Indus Basin in Pakistan using the structure of the hierarchical and multilevel programming model by *Bisschop et al.* [1982]. The solution model employed the transformation matrix approach with 53 irrigated polygonal regions. The original model consisted of 20,000 constraints , but various simplifications reduced the problem to less than 8,000 constraints. A method was developed to this Indus Basin model as a two-level programming problem. One level concerned the farmers and

their individual objectives. The individual farm level objectives were summed and the aggregate farm income was maximised. The second level concerned the government which must account for long-term consequences of water allocation decisions. The solution procedure involved creation of an augmented linear program that served to fix certain policy variables that pertain to government taxes and subsidies.

## 2.14 Groundwater Quality Management

The joint use of numerical simulation and linear programming has been applied to groundwater pollutant source management. The underlying management problem here is the use of an aquifer for both waste disposal and water supply. Combined groundwater simulation and management models have been developed to contend with these problems. Simulation models in the case of groundwater pollutant source management involve solution of the advective-dispersive equation. For the general linear case of a two-dimensional transport with decay and sorption of a single dissolved chemical constituent in saturated porous media, the governing equation may be expressed as

$$R_d \frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left( D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i}(CV_i) - \frac{C'W}{\phi b} - \lambda R_d C \qquad (2.22)$$

where

$C$ concentration in the dissolved chemical species [ $ML^{-3}$ ],

$D_{ij}$ dispersion tensor [ $L^2T^{-1}$ ],

$V_i$ average pore water velocity in the direction $i$ [ $LT^{-1}$ ],

$b$ saturated aquifer thickness [$L$],

$\phi$ effective aquifer porosity [ $L^0$ ],

$C'$ solute concentration in a fluid sink or source [ $ML^{-3}$ ],

$W$ volumetric flux per unit area [ $LT^{-1}$ ],

$R_d$ retardation factor [ $L^0$ ],

$\lambda$ first order kinetic decay rate [ $T^{-1}$ ],

$x_i, x_j$ Cartesian coordinates [$L$], and

$t$ time [$T$].

Different types of management models have been developed for steady state pollution distribution which often represent a worst-case pollution scenario, and for transient cases involving solute redistribution.

### 2.14.1 Steady State Management Models

The first model aimed at managing the disposal of waste in aquifers was that of *Willis* [1976a]. In this study, the aquifer was considered as a component of a regional waste treatment system. The objective of the model was to minimise the cost of surface waste treatment considering both dilution cost and treatment plant cost. The treated effluent would be injected into an aquifer at predetermined sites. Restrictions were place upon water quality at supply wells and recharge wells.

A solute transport model served as a series of linear constraints in the planning model. In the simulation model, no temporal variations could occur in either the hydraulic head or solute distribution. Solute transport simulation proceeded in two steps. First, the steady state form of (2.22) was solved using the finite difference method. The second step

involved determining the steady state solute distribution for each constituent. *Willis* [1976a] chose to neglect dispersion, and modelled on advective transport and adsorption. The finite difference method was again used to discretize the resulting equation for each constituent, and water quality constraints were then based upon these discretized equations. The solute transport simulation model was first formed as a finite difference coefficient matrix. The inverse of this matrix was then computed, and relevant portions were included in the management model as constraints. The management model was demonstrated for a hypothetical case involving two injection wells and two pumping wells. The model considered several unit processes for waste treatment plant that involved primary, secondary, and various forms of advanced waste treatment system. The solution determined the optimal unit treatment process and the most cost-effective volume of imported dilution treated.

Incorporating the discretized solute transport equation as constraints in a linear programming management model was the topic of *Futagami et al.* [1976]. This study considered the general problem of large surface water body pollution and not specifically groundwater pollution. Different models were constructed using finite difference and finite elements to solve for the steady state solute distribution. Their linear programming model sought to maximise total waste disposal under local waste load restrictions. The physical behaviour of the system was accounted for by embedding the finite difference or finite element equations into the linear programming model. The greatest significant of this work was in the linear programming solution algorithm; wherein the author was able to take advantage of the special structure of the constraints represented by the discretized transport equation to develop a more efficient computation algorithm using the simplex method. An initial basic feasible solution was developed without the introduction of artificial variables. However, the primary problem of treating each concentration in space and time as a decision variable still remains, even with their special simplex method implementation.

*Gorelick and Remson* [1982a] and *Gorelick* [1980] employed the embedding approach using the steady state finite difference form of (2.22) to maximise waste disposal at two locations while protecting water quality at supply wells and maintaining an existing waste facility. Both concentration and waste disposal fluxes were treated as decision variables. After achieving the solution, the model was subjected to sensitivity analysis using parametric programming. In this way, waste disposal tradeoffs at the various facilities could be inspected.

### 2.14.2 Transient Management Models

Pollutant source management problems may frequently involve the migration of plumes of contaminated water. In such cases, water quality must be protected over long time frames. A waste disposal decision today may not manifest itself as polluted groundwater at down-gradient wells or streams for many decades. Methods to contend with the dynamic management of groundwater pollutant sources have therefore been developed.

Both *Willis* [1976b] and *Futagami* [1976] suggested that the embedding method be employed using the finite element formulation of the solute transport model to solve the transient management problem. *Willis* [1976c] employed the embedding method to determine effluent disposal standards for food processing waste using spray irrigation. His finite element model considered one-dimensional advective and dispersion for five disposal cycles for a 24-element configuration. For such small system, the embedding method is applicable. However, for a general transient case, the embedding method will result in an extremely large constraint matrix making the embedding approach unsuitable.

*Gorelick et al.* [1979] considered the management of a transient pollutant source. Their model determined the maximum permissible concentration in a river which lost water to an aquifer. They recognised the problem of storing and manipulating a large time- and

space-discretized matrix when using the embedding approach and developed an alternate method. This method did not require linear programming. By taking advantage of the mathematical structure of the transient constraints matrix, a recursive pollutant source management problem was developed. Concentration throughout the system was expressed as a function of the river water quality. The management solution was quite different and provided valuable information regarding the effect of successive water quality constraints, as well as travel times of the solute plume peaks from the source to the location of the supply wells. This method is however, limited to situations in which the concentration of the system can be expressed as a function of a single parameter.

*Willis* [1979] considered a model for aquifer management involving waste injection control. He considered the groundwater problems associated with the well injection of waste waters in a groundwater aquifer system conjunctively managed for supply and quality. The planning problem was broken into groundwater hydraulic management, and pollutant source management components. By decomposing the problem in this manner, the hydraulic heads as determined from the hydraulic management solution, were used to generate the groundwater velocity field required for the groundwater quality management model. The two component problems were formulated and solved as separate linear programming problems. In an illustrative example, hydraulic heads were managed at extraction and injection wells while a water target within each planning period was met and pumping and injection rates were limited. The water quality component maximised the lowest of the waste injection concentrations while meeting a waste disposal load and preserving water quality at all wells during the operational cycle. The example considered four 120-day management periods. Decisions regarding pumping and injection were made at the beginning of each period. Transient hydraulic simulations were avoided by using an average groundwater velocity field over the 480-day operational cycle for the water quality simulation-management model.

Each of the two management models predicted the system's behaviour using numerical simulation. To handle the question of dimensionality associated with transient problems, *Willis* [1979] began by constructing finite element models for the flow and solute transport models. Rather than discretizing the time derivatives, the system was discretized over space alone. Analytic solutions to these systems of space-discretized ordinary differential equations were obtained [*Bellman*, 1960] and the solutions were entered into the linear programming models as constraints. For the water quality subproblem, there are some difficulties with this approach. First, evaluating concentrations at the beginning and end of a planning period does not suffice. In transient problems, decisions are made regarding levels of waste water disposal at potential sites. The optimal selection of sites and waste disposal strengths are unknown, and therefore the arrival time of contaminant plume peaks at water supply wells remains unknown. Contaminant plumes will not arrive at each supply well at the beginning or end of a planning period. Second, numerical problems may arise when solving the solute transport equation as a system of ordinary differential equations. This is because the space-discretized equations for a nonsymmetric matrix are difficult to solve using the matrix exponential.

*Gorelick and Remson* [1982b] approached the dynamic management of groundwater pollutant sources by the use of a constraint response matrix. They considered an illustrative one dimensional case involving multiple sources of groundwater pollution and the maintenance of water quality at water supply wells over all time. They were concerned with the problem of managing waste disposal activities for several years in such a way that solute concentration at supply wells never exceed water quality standards, even after waste disposal activities had ceased. An external finite difference model was used to construct a unit source concentration response matrix. The matrix served as linear programming constraints and converted solute injected fluxes at potential disposal locations into concentration histories at water supply wells. Any linear solute transport simulation model could be used to generate the concentration response matrix. The linear programming

solution was subjected to parametric programming to analyse the influence upon the optimal solution of various waste injection strategies.

*Gorelick* [1982] utilised the U.S. Geological Survey method of characteristics solute transport model [*Konikow and Bredehoeft*, 1978] as a component in a groundwater quality management model applied to a complex hypothetical regional aquifer. The concentration response matrix was used in conjunction with linear programming to maximise waste disposal at several facilities during 1-year planning periods. A limit on solute concentration at observation wells was enforced from the first arrival of groundwater pollution until the pollutant plumes cleared the observation wells. He found that by formulating the problem as a dual linear programming problem and by using a numerically stable implementation of the revised simplex method [*Saunders*, 1977], a large field-scale problem could be solved. The results of the pollutant source maximisation problem indicated that the waste disposal was enhanced by pulsing rather than maintaining constant disposal rates at various sites. Solutions to problems with successfully greater numbers of waste disposal periods were compared. The marginal impact of the water quality standard imposed at the supply wells was greater for short management horizons than for extended management horizons.

*Gorelick and Remson* [1982b] and *Gorelick* [1982] were concerned with managing disposal decisions until the pollutants essentially cleared the system. This differs from the water quality problem of *Willis* [1979] in which the disposal cycle and the time during which groundwater pollution was of concern were synonymous. Furthermore, the advantage of solving the space-discretized form of the solute transport model using an analytic solution lies in the ability to obtain a solution at any arbitrary time rather than at successive discrete times. If analytic solutions are obtained over discrete time intervals in order to ensure water quality at supply wells over the entire problem time frame, then the primary benefit of the analytic solution technique is lost. In addition, incorporating transient field flow variations would require numerous evaluations of matrix exponentials at discrete times. In the case considered by *Gorelick and Remson* [1982b] and *Gorelick* [1982],

pollutant plume peaks arrived over a span of years and at different unknown times at the various supply or observation wells. Temporal flow field variations could be incorporated by the sequential solution of the flow and transport models when developing the concentration response matrix and use of the concentration response matrix is not restricted to a particular simulation model. Any simulation model may be used to generate the concentration response matrix, as demonstrated by *Gorelick* [1982].

### 2.14.3 Some Current Groundwater Management Studies

*Dougherty and Marryott* [1991] showed that simulated annealing can be applied effectively to optimise problems in groundwater management. Simulated annealing is a probabilistic optimisation method that can work well for large scale optimisation problems that are cast in discrete or combinatorial form. The basic simulated annealing algorithm uses a random search technique for locating candidate solutions (or configurations) and a probabilistic criterion for accepting or rejecting those solutions that will not lead to improved configurations. The method derives its name from an analogy with the way solids anneal into a highly ordered (ie., optimal) structure. Their objective was to formulate the problem in terms of a discrete number of decision variables, each with a discrete number of possible values. Simulated annealing was then applied to the resulting combinatorial problem. The combinatorial problem has a finite, though potentially large, number of possible solutions. A solution that results in the 'best' or globally optimal value of the objective function is nonunique. They indicated that in theory simulated annealing can guarantee a global optimum but noted that in practice, computational limitations leads to the search for nearly optimal solutions.

*Marryott et al.* [1993] used simulated annealing to analyse alternate design strategies for a groundwater remediation at a contaminated field site through a combination

of the simulated annealing optimisation algorithm with a field-scale flow and solute transport simulation model for an unconfined aquifer. Their objective was to determine nearly optimal pumping schedules for a pump-and-treat remediation system at a proposed Superfund site in central California. They presented a series of demonstration problems using two different optimisation formulations. The results of their experiment indicated that the simulated annealing method can be applied to realistic groundwater management problems. However, they also noted that the computational expense of simulated annealing technique is large but comparable to other nonlinear optimisation techniques. They finally provided a practical empirically based strategy for selecting and adjusting the parameters necessary for successful optimisation.

*Andricevic and Kintanidis* [1990] presented the approximate dual-control method in which the policy improves the estimation of system parameters as well as manages the system to meet the specified objectives of minimal cost (remediation). Using small perturbation theory, the objective function was divided into a deterministic and stochastic components. Differential dynamic programming was used to compute the deterministic control. The solution for the stochastic part of the objective function was obtained by analytic calculation. Because of this feature, computation requirements did not exhibit the dimensionality problem associated with the conventional discrete stochastic dynamic programming. For on-line parameter identification, the extended Kalman filter was used to update the state estimates and state covariances. The methodology was applied to a hypothetical one-dimensional bounded aquifer system and did not account explicitly for inequality constraints.

Convinced that it is practically impossible to specify processes and parameters precisely in a remediation design program, *Lee and Kitanidis* [1991] presented the method of optimal estimation and scheduling in aquifer remediation with incomplete information. Their methodology combines computer simulation models of solute transport and fate, descriptions of spatial variability, probabilistic analysis of uncertainty, and optimisation.

Their objective was to identify the most cost effective management policy. They noted that the advantages of their technique included : (1) utilisation of measurements in real time, (2) simultaneous estimation of aquifer parameters and decisions for remediation, and (3) provision of a more diversity in cost-effectiveness and decisions for aquifer remediation. Subject to constraints and for a given reliability of meeting water quality standards, their method minimises the expected value of the cost in the remaining periods. Because of incomplete information about the site, the cost of decontamination strategy is not known a priori. Hence, their objective minimises the cost weighted by the probability that it will be incurred.

The optimal aquifer management policy is expressed as the sum of the deterministic and a stochastic control term. The former is obtained by solving a deterministic optimisation problem through constrained differential dynamic programming, and the latter is obtained by a perturbation approximation to the stochastic optimal control problem. Extended Kalman filtering is incorporated into the optimisation method to improve the accuracy of the estimated state and parametric variables using available measurements. A hypothetical contamination case with two-dimensional unsteady flow and transport for a persistent solute was used to illustrate the applicability of their methodology. The cost effectiveness and reliability of the proposed method was studied under various conditions and then compared with the cost and reliability of the deterministic feedback control method through Monte Carlo simulation. They noted that their methodology, which posed as an extended case of *Andricevic and Kitanidis* [1990] in two-dimensional aquifer with spatial variability in parameter and various constraints, was superior to the deterministic feedback control.

*McKinney and Lin* [1994] used a genetic algorithm to solve a mixed integer nonlinear program optimal remediation design problem that included fixed and variable treatment and well field costs. They noted that their formulation of the problem with genetic algorithm was straightforward and provided solutions which were as good or better than those obtained by linear and nonlinear programming. Their technique however, did not

account for the possibility of extraction well redundancy as a contaminant plume moves along with time. Accounting for the possibility of extraction well redundancy is important since over-estimation of remedial design cost can be avoided as contaminant plume move from the operating extraction wells. They indicated in their work that complicated problems, such as transient pumping and multiphase remediation which have proved difficult for the embedding and response matrix approaches of linear and quadratic programming could be readily formulated and solved without essential difficulties. Constraints could be easily incorporated into the formulation and computation of derivatives with respect to the decision variables (as in nonlinear programming) were not required. However, they mentioned that the computational time required for the solution of genetic algorithm groundwater management models increases with the complexity of the problem. They noted that for such complicated problems, the computational time could be dramatically reduced on massively parallel computers.

*Ritzel and Eheart* [1994] have also employed the genetic algorithm technique to solve a multiple objective groundwater pollution containment problem. Their purpose was to investigate the ability of the genetic algorithm to solve a multiple objective groundwater pollution problem. Their method involved operating a set of wells so that the polluted water could be hydraulically contained and can be pumped for subsequent treatment. Their decision variables were how many wells to install, where to install them, and how much to pump from each well. To achieve this, they formulated two methods with the genetic algorithm: a vector-evaluated genetic algorithm and a Pareto genetic algorithm. However, since their model was only concerned with steady-state groundwater pollution containment, and not groundwater remediation, contamination transport was not considered in their studies. They concluded in their work that genetic algorithms are capable of generating trade-off curves for a multiple objective groundwater containment problem and mentioned that one great advantage of the genetic algorithm over conventional optimisation lies in its ability to handle highly nonlinear complex problems that accurately reflect the real world.

## 2.15 Approach in Present Research

In the second part of this research work, a complete groundwater optimisation model has been proposed for remediation of polluted aquifers. A comprehensive literature survey has presented a numerous number of previous and current techniques that have been used for such exercises. The previous techniques mostly deal with linear and nonlinear methods that employ embedding and response matrix deterministic methods. The disadvantages of these methods lie in their inability to handle large and complex real problems. Not surprisingly, such methods are not adopted in the techniques of the '90s where more sophisticated methods such as simulated annealing, stochastic, and a combination of deterministic and stochastic techniques are now in use.

Nonlinear programming techniques have been used to solve groundwater management problems for the past two decades. These methods employ the gradient-based algorithms to adjust decision variables so as to optimise the objective function of a management model. These algorithms require the computation of sensitivities of state variables, eg., head or concentration, at certain locations to decision variables. Sensitivities are obtained either by adjoint sensitivity or perturbation methods. These sensitivities are difficult to program, in the case of adjoint sensitivity method, or computationally expensive to generate, in the case of perturbation methods, and in general are not robust [*McKinney and Lin*, 1994]. The problem is complicated by the fact that cost functions may either be discontinuous or highly complex. Additionally, groundwater management problems tend to be highly nonlinear and nonconvex mathematical programming problems, especially in the case of aquifer remediation design with mass transport constraints. Hence, there is no

guarantee that a global optimum of a groundwater remediation design will be found by gradient-based nonlinear programming methods.

Genetic algorithms are search algorithms based on the principle of the mechanics of natural selection which are capable of finding several near-optimal design alternatives that are different from each other - giving the decision maker several alternatives to compare and select from. Therefore in view of the several inherent difficulties associated with the use of nonlinear programming methods to the design of groundwater remediation schemes, the genetic algorithm technology has been selected as the suitable method for application in the proposed remediation model of the second phase of this research work. The details of this technique and the extent to which it is formulated to suit the needs of this research study is presented in chapter five. It is apparent from the literature survey, that the shuffled complex evolutionary (SCE) method has never been used in the history of groundwater modelling for parameter estimation. This technique has proved very successful in the past for the calibration of conceptual surface runoff models. In the light of its success, it has been selected as the technique to be adopted in the inverse problem of parameter estimation. Details of the SCE methodology is presented in chapter five.

## 2.16 Summary

This chapter has presented a comprehensive review of the various methodologies used in the optimisation of groundwater management and aquifer parameter identification problems. The topics discussed range from the application of deterministic (gradient-based methods) through a combination of deterministic and stochastic methods (shuffled complex evolution) to completely stochastic methods (simulated annealing and genetic algorithms). Current research studies have shown that gradient-based methods have difficulties in locating the global optimum of the objective function of groundwater management

problems. However, they have indicated that techniques like the genetic algorithm and the shuffled complex evolution methods are robust enough to handle most of the difficulties associated with real-world complex optimisation problems. In view of this, the genetic algorithm and the shuffled complex methodology have been selected as the appropriate optimisation techniques for proposed aquifer remediation and the parameter estimation in this research study.

# Chapter 3

# Research Methodology

## 3.1 Introduction

Based on the comprehensive literature survey presented in chapter 2, two appropriate evolutionary techniques have been selected to handle the two-phase research study proposed in the introductory chapter. The first phase of the research study deals with the identification of aquifer formation parameters using the shuffled complex evolutionary methodology, while the second phase considers the optimisation of extraction processes in contaminated aquifers using the genetic algorithm optimisation technique. The shuffled complex evolution and the genetic algorithm are both evolutionary optimisation techniques that employ the principles of natural selection. The outstanding difference between the two is that the genetic algorithm uses entirely stochastic (or probabilistic) methods in its optimisation procedures while the shuffled complex evolution combines both stochastic and deterministic methods. In both phases of the research study, numerical finite element models are embedded in the optimisation models for the forward problem part of the analysis. This chapter briefly addresses the approach adopted in the development of the desired models for each phase of the proposed research.

## 3.2 Parameter Identification - Phase 1

In order to design a more practical tool for field scale problems, numerical formulation techniques are adopted to solve the governing equations of flow and solute transport. Two stand-alone models (one for flow and the other for solute transport) each with the option to handle fluid flow in both two- and three-dimensions are designed for the inverse problem of parameter identification. The optimiser used in this model is the shuffled complex evolutionary technique. The shuffled complex evolution (SCE) performs the entire parameter estimation operation through two major operations: (1) complex shuffling, and (2) competitive complex evolution. Importance is attached to the estimation of the following parameters:

*Two-Dimensional Flow model*

- hydraulic conductivity in the x-direction [ $k_{xx}$ ],
- hydraulic conductivity in the y-direction [ $k_{yy}$ ],
- anisotropic hydraulic conductivity [ $k_{xy} = k_{yx}$ ], and
- aquifer storage coefficient [$S$]

*Three-Dimensional Flow model*

- hydraulic conductivity in the x-direction [ $k_{xx}$ ],
- hydraulic conductivity in the y-direction [ $k_{yy}$ ],
- hydraulic conductivity in the z-direction [ $k_{zz}$ ], and
- aquifer storage coefficient [$S$].

*Two- and Three-Dimensional Transport Models*

- longitudinal dispersivity [ $\alpha_L$ ],
- transverse dispersivity [ $\alpha_T$ ], and
- aquifer porosity [ $\phi$ ].

Nonuniformity and nonhomogeneity are accounted for in groundwater modelling via: (1) zonation method, and (2) interpolation method. In the zonation approach, the simulation region is divided into a number of subregions (or zones) and constant parameter value are used to characterise each zone. In the finite element context therefore, all elements within the same zone exhibit common parameter values corresponding to that zone. Parameter identification numbers are used to parameterize the region into zones. Therefore elements identified by the same numbers are known to belong to the same zone and hence have common parameter values. In the interpolation approach, the simulation region is divided into a number of elements connected to a number of nodes. Each node is associated with a chosen local interpolation function. The unknown parameter is then interpolated by a linear combination of the interpolating function. Because of its ease of application, the zonation method is adopted in this research work to account for nonuniformity and nonhomogeneity of the aquifer formation parameters.

The decision to use the SCE for the inverse problem of parameter identification is based on the considerable amount of success which some surface hydrologists have reported on its use for calibration of conceptual rainfall-runoff (CRR) models. Recently, *Tanakamaru and Burges* [1996] and *Kuczera* [1997] compared the efficiency of the SCE technique in the context of CRR modelling with the genetic algorithm and other optimisation techniques and reported the SCE as having the best performance. *Yapo et al.* [1996] used a 39 water-year period in conjunction with the SCE to estimate the optimal parameters of a given watershed. They performed ten independent runs and concluded that all the ten runs

converged to the same parameter values. Additionally Professor H. Gupta - the leader of the team that developed the shuffled complex evolutionary technique - has mentioned in a personal communication that the methodology has never been extended to groundwater modelling. Therefore the primary objective of the use of the SCE in the inverse problem of parameter identification is to investigate its performance in the context of groundwater modelling.

## 3.2 Optimisation of Extraction - Phase 2

This model comprises a flow and solute transport model embedded in the genetic algorithm optimisation model. The flow model is required for the computation of element centroidal velocities which is subsequently used in the transport model for the computation of dispersion coefficient parameters. In addition to handling anisotropy and homogeneity, the numerical models in this context are designed to model fluid transport processes in confined and unconfined aquifers. The major task of the optimisation is performed by the genetic algorithm model through the four genetic processes of selection, crossover, mutation, and inversion; after receiving nodal concentration values from the transport model. The nodal concentration values are required by the genetic algorithm for the evaluation of the objective function. The output of the entire optimisation process is (1) the optimum number, locations, pumping rates, and pumping regime of extraction wells and (2) the optimum cost of the extraction operation associated with the entire remediation scheme in (1).

## 3.4 Assumptions

Since mathematical models are not completely capable of simulating the realities of nature, assumptions are usually required in some cases to reduce the complex natural phenomena to situations that can be readily modelled. In view of this, the following assumptions are observed by the flow and solute transport governing equations adopted in this research work.

### 3.4.1 Major Assumptions of the Flow Models

- Flow of the fluid is considered isothermal and governed by Darcy's law,
- fluid under consideration is slightly compressible and no separation phase occurs, and
- the daughter products of any decayed material do not affect the density of water.

### 3.4.2 Major Assumptions of the Transport Models

- Diffusion of transport in the porous medium is governed by Fick's law,
- the hydrodynamic dispersion is defined as the sum of the coefficient of mechanical dispersion and molecular diffusion,
- adsorption and decay of the solute may be described by a linear equilibrium isotherm and a first-order decay rate, and
- decay rate is the same in both the solid and the liquid phase.

## 3.5 Formulation and Numerical Approximation

In the usual finite element context, the steps involved in the formulation and numerical approximation consist of:

- Discretization of the simulation region into a network of finite elements. For simple rectangular simulation regions, subprograms have been designed and incorporated for automatic generation of element connectivity and nodal coordinates (mesh design).
- Formulation of a matrix equation describing the behaviour of individual elements (element stiffness matrix). The weighted residual of the advective-dispersive transport is performed using asymmetric weighting functions (instead of the basis functions normally used in the standard Galerkin formulation). This measure is effected to take care of numerical dispersion when the advective components of the transport model dominate over their dispersive counterparts. This upstream-weighting technique is adopted in the management model.
- Assembly of the element equations into a system of global algebraic equations and incorporation of boundary conditions.
- Solution of the resulting system of algebraic equations using a direct symmetric solver for the flow model and a direct asymmetric solver for the transport model of the management model. An iterative solution technique is used for the inverse problem of parameter identification for fast solution process since some problems require a large number of objective function evaluations.

## 3.6 Summary

A brief methodology of the proposed research study has been presented in this chapter. The entire research work comprises two phases. The first phase involves the development of a model for the inverse problem of parameter identification using the shuffled complex evolutionary methodology. The second phase deals with the development of a management model for the optimisation of extraction processes in polluted aquifers using the genetic algorithm as the optimisation technique. Within each of these optimisation models, is embedded a flow and/or solute transport model. These models are formulated by the finite element method into a system of algebraic equations which are solved appropriately by direct and iterative solution techniques. Details of the optimisation models mentioned in this chapter and the extent to which they are formulated to handle the proposed problem presented in chapter five. The governing equations, their numerical formulation into a system of algebraic equations, and solution techniques used to solve these system of algebraic equations are presented in much more detail in chapter four.

# Chapter 4

# Governing Equations, Finite Element Formulation, and Solution Techniques

## 4.1 Introduction

This chapter addresses the equations governing flow and solute transport in porous media, their subsequent formulation into a system of algebraic equations by the finite element method, and the appropriate solution techniques employed to solve the system of algebraic equations. From the methodology presented in chapter three, a total of four governing equations are presented. These are namely: (1) a two-dimensional flow equation, (2) a three-dimensional flow equation, (3) a two-dimensional solute transport equation and (4) a three-dimensional solute transport equation. In the proposed extraction process, a flow model is required for the computation of velocities to be used by the solute transport component of the extraction model. The presentation of these equations are followed by their transformation into a system of algebraic equations using the finite element method.

## 4.2 Governing equations for the Flow Models

The generalised anisotropic and nonhomogenous form of governing equations for a two-dimensional flow model may be expressed as:

$$\frac{\partial}{\partial x}\left(k_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial x}\left(k_{xy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial y}\left(k_{yx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_{yy}\frac{\partial h}{\partial y}\right)=S\frac{\partial h}{\partial t}+Q \qquad (4.1)$$

where:

| | |
|---|---|
| $k_{xx}$ | hydraulic conductivity in the x-direction [ $LT^{-1}$ ], |
| $k_{xy}$ | anisotropic hydraulic conductivity in xy-direction [ $LT^{-1}$ ], |
| $k_{yx}$ | anisotropic hydraulic conductivity in the yx-direction [ $LT^{-1}$ ], |
| $k_{yy}$ | hydraulic conductivity in the y-direction [ $LT^{-1}$ ], |
| $h(x,y,t)$ | hydraulic head at a point (x,y) at time $t$ [$L$], |
| $t$ | a particular simulation time [$T$], |
| $Q$ | volumetric rate of extraction/injection per unit area [ $LT^{-1}$ ], and |
| $S$ | aquifer storage coefficient [ $L^0$ ]. |

The three-dimensional from of equation (4.1) may be expressed as:

$$\frac{\partial}{\partial x}\left(k_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(k_{zz}\frac{\partial h}{\partial y}\right)=S\frac{\partial h}{\partial t}+Q \qquad (4.2)$$

$$k_{xy}=k_{yx}=k_{yz}=k_{zy}=k_{xz}=k_{zx}=0$$

where:

| | |
|---|---|
| $k_{zz}$ | hydraulic conductivity in the vertical (or z) direction [ $LT^{-1}$ ]. |

All other terms in equation (4.2) have meanings as previously defined in equation (4.1). In the finite element formulation, it is rather convenient to have equations (4.1) and (4.2) in their Cartesian tensor notation form. Using this notation, equations (4.1) and (4.2) may be represented in a more compact form as:

$$\frac{\partial}{\partial x_i}\left(k_{ij}\frac{\partial h}{\partial x_j}\right) = S\frac{\partial h}{\partial t} + Q, \qquad (4.3)$$

$i, j = 1,2$ (for 2 - dimension) or $i, j = 1,2,3$ (for 3 - dimension)

where:

$k_{ij}$ hydraulic conductivity tensor [$LT^{-1}$].

$k_{ij}$ contains the diagonal elements $k_{xx}$ and $k_{yy}$ and the off-diagonal terms $k_{xy}$ and $k_{yx}$ for the two-dimensional model or $k_{xx}$, $k_{yy}$, and $k_{zz}$ for the three-dimensional model (where all other elements of hydraulic conductivity tensor are zero). In accordance with the standard definitions, transmissivity may be obtained from the hydraulic conductivity tensor by the expression:

$$T_{ij} = k_{ij} H \qquad (4.4)$$

where:

$T_{ij}$ transmissivity tensor [$L^2T^{-1}$], and

$H$ saturated thickness of the aquifer [$L$].

For unconfined flow, $H$ corresponds to the hydraulic head above the base of the aquifer. The initial and boundary conditions to which equation (4.3) may be subject to are expressed as:

$$h(x_i, t = 0) = h_0 \qquad (4.5)$$

$$h(x_i, t) = \bar{h} \quad \text{on boundary } B_1 \qquad (4.6)$$

$$-k_{ij}\frac{\partial h}{\partial x_j}n_i = q \quad \text{on boundary } B_2 \qquad (4.7)$$

where:

$h_0$ initial hydraulic head [$L$],

$\bar{h}$ specified hydraulic head on boundary portion $B_1$ [$L$],

$q$ specified flux on boundary portion $B_2$ [$LT^{-1}$], and

$n_i$ outward unit normal vector.

## 4.2 Governing equations for the Transport Models

The two-dimensional governing equation for solute transport in a porous medium may be represented by the mathematical expression:

$$\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}+D_{xy}\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial y}\left(D_{yx}\frac{\partial c}{\partial x}+D_{yy}\frac{\partial c}{\partial y}\right)-v_x\frac{\partial c}{\partial x}-v_y\frac{\partial c}{\partial y}= R\frac{\partial c}{\partial t}+R\lambda c+\frac{Q_f}{\phi m}\left(c^*-c\right) \tag{4.8}$$

where:

$D_{xx}$ hydrodynamic dispersion coefficient in the x-direction [$L^2T^{-1}$],

$D_{xy}$ hydrodynamic dispersion coefficient in the xy-direction [$L^2T^{-1}$],

$D_{yx}$ hydrodynamic dispersion coefficient in the yx-direction [$L^2T^{-1}$],

$D_{yy}$ hydrodynamic dispersion coefficient in the y-direction [$L^2T^{-1}$],

$c(x,y,t)$ trace concentration at the point (x,y) in time $t$ [$ML^{-3}$],

$v_x$, $v_y$ pore water velocities in x- and y-directions, respectively [$LT^{-1}$],

$R$ retardation coefficient [$L^0$],

$\lambda$ decay constant [$T^{-1}$],

$Q_f$ injection (or extraction) rate per unit area [$LT^{-1}$],

$c^*$ trace concentration in injected fluid [$ML^{-3}$],

$\phi$ aquifer porosity [ $L^0$ ], and

$m$ aquifer saturated thickness [$L$].

The hydrodynamic dispersion components are evaluated according to the following constitutive relations [*Istok*, 1987]:

$$D_{xx} = \frac{\alpha_T v_y^{\,2} + \alpha_L v_x^{\,2}}{v} + D^* \tag{4.9}$$

$$D_{yy} = \frac{\alpha_T v_x^{\,2} + \alpha_L v_y^{\,2}}{v} + D^* \tag{4.10}$$

$$D_{xy} = D_{yx} = \frac{(\alpha_L - \alpha_T) v_x v_y}{v} \tag{4.11}$$

where:

$$v = \left| \sqrt{v_x^{\,2} + v_y^{\,2}} \right|$$

$\alpha_L$ longitudinal dispersivity [$L$],

$\alpha_T$ transverse dispersivity [$L$], and

$D^*$ coefficient of molecular diffusion [ $L^2T^{-1}$ ].

The three-dimensional form of the solute transport model in equation (4.8) may be expressed as:

$$\begin{aligned} &\frac{\partial}{\partial x}\left( D_{xx}\frac{\partial c}{\partial x} + D_{xy}\frac{\partial c}{\partial y} + D_{xz}\frac{\partial c}{\partial z}\right) + \frac{\partial}{\partial y}\left( D_{yx}\frac{\partial c}{\partial x} + D_{yy}\frac{\partial c}{\partial y} + D_{yz}\frac{\partial c}{\partial z}\right) + \\ &\frac{\partial}{\partial z}\left( D_{zx}\frac{\partial c}{\partial x} + D_{zy}\frac{\partial c}{\partial y} + D_{zz}\frac{\partial c}{\partial z}\right) - v_x\frac{\partial c}{\partial x} - v_y\frac{\partial c}{\partial y} - v_z\frac{\partial c}{\partial z} = R\frac{\partial c}{\partial t} + R\lambda c + \frac{Q_f}{\phi m}\left(c^* - c\right) \end{aligned} \tag{4.12}$$

where:

$D_{xz}$ hydrodynamic dispersion coefficient in the xz-direction [ $L^2T^{-1}$ ],

$D_{zx}$ hydrodynamic dispersion coefficient in the zx-direction [ $L^2T^{-1}$ ],

$D_{yz}$ hydrodynamic dispersion coefficient in the yz-direction [ $L^2T^{-1}$ ],

$D_{zy}$ hydrodynamic dispersion coefficient in the zy-direction [ $L^2T^{-1}$ ],

$D_{zz}$ hydrodynamic dispersion coefficient in the z-direction [ $L^2T^{-1}$ ], and

$v_z$ pore water velocity in the z-direction [ $LT^{-1}$ ].

All the other parameters in equation (4.12) have the same meaning as those defined in equation (4.8). The expressions for the coefficients of mechanical (or hydrodynamic) dispersion in three-dimensional notation may be obtained by the following expression [*Istok*, 1987]:

$$D_{xx} = \frac{\alpha_T\left(v_y^{\,2} + v_z^{\,2}\right) + \alpha_L v_x^{\,2}}{v} + D^* \tag{4.13}$$

$$D_{yy} = \frac{\alpha_T\left(v_x^{\,2} + v_z^{\,2}\right) + \alpha_L v_y^{\,2}}{v} + D^* \tag{4.14}$$

$$D_{zz} = \frac{\alpha_T\left(v_y^{\,2} + v_x^{\,2}\right) + \alpha_L v_z^{\,2}}{v} + D^* \tag{4.15}$$

$$D_{xy} = D_{yx} = \frac{(\alpha_L - \alpha_T)v_x v_y}{v} \tag{4.16}$$

$$D_{xz} = D_{zx} = \frac{(\alpha_L - \alpha_T)v_x v_z}{v} \tag{4.17}$$

$$D_{yz} = D_{zy} = \frac{(\alpha_L - \alpha_T)v_z v_y}{v} \tag{4.18}$$

where

$$v = \left|\sqrt{v_x^{\,2} + v_y^{\,2} + v_z^{\,2}}\right|$$

In Cartesian tensor notation equations (4.8) and (4.12) may be expressed in a more compact form as:

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c}{\partial x_j}\right) - v_i\frac{\partial c}{\partial x_i} = R\frac{\partial c}{\partial t} + R\lambda c - \frac{Q_f}{m\phi}(c^* - c) \qquad (4.19)$$

$$i,j = 1,2 \text{ (2 - dimension) or } i,j = 1,2,3 \text{ (3 - dimension)}$$

where:

$D_{ij}$ hydrodynamic dispersion tensor [$L^2T^{-1}$].

The elements of $D_{ij}$ are the hydrodynamic dispersion coefficients defined in equations (4.9) to (4.11) and in equations (4.13) to (4.18) for the two- and three-dimensional models, respectively. The initial and boundary conditions associated with the solution of equation (4.19) may be expressed as:

$$c(x_i, t = 0) = c_0 \qquad (4.20)$$

$$c(x_i, t) = \bar{c} \quad \text{on boundary } B_1 \qquad (4.21)$$

$$v_i n_i c - k_{ij}\frac{\partial c}{\partial x_j}n_i = q_f c_f \quad \text{on boundary } B_2 \qquad (4.22)$$

where:

$c_0$ initial tracer concentration [$ML^{-3}$],

$\bar{c}$ specified concentration at boundary portion $B_1$ [$ML^{-3}$], and

$q_f c_f$ specified concentration flux at boundary portion $B_2$ [$ML^{-3}T^{-1}$].

The compact forms of the governing equations discussed so far for the 2- and 3-dimensional flow and solute transport models are shown in equations (4.3) and (4.21), respectively. These equations are in partial differential equation form, therefore for the dependent variables to be evaluated, they must be reduced to a system of algebraic equations by one of the known numerical formulation techniques.

## 4.3 Numerical Formulation Techniques

Numerical formulation techniques are methods used to reduce the governing equations (containing partial differential expression) to a system of solvable algebraic equations. Numerical methods do not require such restrictive assumptions as those required by the closed-form solutions of analytical models. For example, it is possible to obtain numerical solutions for the case of anisotropic and nonhomogenous aquifer properties and for problems with complex and time-dependent boundary conditions. In using numerical methods, one seeks a discrete approximation for the solution, ie., computed values of the field variable at a set of specified points within the aquifer at a set of specified times. The number and locations of the points and the number and choice of time steps are determined in advance by the analyst. Several types of numerical methods have been used to solve groundwater flow and solute transport problems in the past. The two principal ones are the Finite Difference Method (FDM) and the Finite Element Method (FEM).

The FDM was initially applied to groundwater flow of fluids in petroleum reservoirs as far back as the early '50s [*Bruce et al.*, 1953, *Peaceman and Rachford*, 1962], and later to problems of groundwater flow and solute transport in the mid-1960's [*Remson et al.*, 1965; *Freeze and Whitherspoon*, 1966; *Pinder and Bredehoeft*, 1968]. The FDM has a number of advantages that has contributed to its continued widespread use and popularity: (1) for simple problems, the mathematical formulation and computer implementation are easily understood by those without advanced training in mathematics or computer programming, (2) efficient numerical algorithms have been developed for implementing the FDM on computers, (3) the accuracy of solutions to steady-state and transient groundwater flow problem is generally quite good, and (4) several case histories

have been published that describe successful application of the method to the solution of practical problems. Unfortunately the FDM has some disadvantages: (1) the method works best for rectangular or prismatic aquifers of uniform composition; it is difficult to incorporate irregular or curved aquifer boundaries, anisotropic and heterogenous aquifer properties, or sloping soil and rock layers into the numerical model without introducing numerous mathematical and computer programming complexities, and (2) the accuracy of the solution to transport problems is lower than can be obtained for the FEM (which is now widely used in place of the FDM for this purpose).

The FEM was first used to solve groundwater flow and solute transport in the early 1970's [*Zienkiewicz et al.*, 1966; *Javadel and Witherspoon*, 1968; *Zienkiewicz and Parekh*, 1970; *Pinder and Frind*, 1972]. Some of the advantages of the FEM are : (1) irregular or curved aquifer boundaries, anisotropic and heterogenous aquifer properties, and sloping soil or rock layers can be easily incorporated into the numerical model, (2) the accuracy of solutions to groundwater flow and solute transport problems is very good (exact in some cases), (3) solutions to the solute transport equation are generally more accurate than those obtained by the FDM, and (4) the FEM lends itself to modular computer programming wherein a wide variety of problems can be solved using a small set of identical computer procedures. The FEM however has certain disadvantages: (1) for very simple problems, the FEM requires a greater amount of mathematical and computer programming sophistication than does the FDM (although this disadvantage disappears for more complicated problems), and (2) unlike the FDM which can be represented using Taylor's series, the theory behind the FEM is relatively abstract and difficult to understand by beginners. However, the advantages of the FEM appears to outweigh its disadvantages especially in the event of complex anisotropic and nonhomogenous aquifers with irregular boundary geometry. In view of the capabilities of the FEM to handle such complex problems, it is has been selected as the appropriate

numerical formulation technique for the governing equations of flow and solute transport presented in section 4.2.

### 4.3.1 FEM Formulation of the Flow Model

FEM formulation techniques such as the Galerkin method and the variational principle have been used in the past to formulate governing equations into a system of solvable algebraic equations. The variational principle, which uses the concept of energy dissipation, works only for some particular equations (for example, it is incapable of handling the solute transport model because of the advective component in the governing equation). The standard Galerkin FEM is general for all governing equations since it derives its methodology from the method of weighted residuals. Because of its generality, the Galerkin FEM is employed in the formulations of the governing equations discussed previously. The formulation presented below is applicable to both two- and three-dimensional governing equations. The first step is to define an approximate or trial solution $h_{tr}(x_i,t)$, as a series summation in terms of the unknown head $h(x_i,t)$ and an interpolating function, $N_J(x_i)$, such that,

$$h_{tr}(x_i,t) = N_J(x_i)h(t), \qquad J = 1,2,..,n \tag{4.23}$$

where $n$ is the number of nodes in the entire finite element network. Substitution of the trial solution into a given governing equation results in residuals (or errors) at each nodal point. If a particular average of the weighted residual is forced to vanish, the nodal heads are obtained as the solution of the system of algebraic equations - this is the basis of the Galerkin FEM formulation. The details of the technique can now be applied to equation

(4.3). Substitution of the trial solution into equation (4.3) yields the residual $\varepsilon(x_i,t)$ which may be expressed as:

$$\frac{\partial}{\partial x_i}\left(k_{ij}\frac{\partial h_{tr}}{\partial x_j}\right) - S\frac{\partial h_{tr}}{\partial t} - Q, \; = \varepsilon(x_i,t) \tag{4.24}$$

The residual $\varepsilon(x_i,t)$ is forced to vanish by weighting it with a weighting function *w*, and summing over the entire simulation domain. In the Galerkin formulation technique, the weighting function *w*, is considered as the interpolating (or shape) function $N_I(x_i)$. This weighting operation results in the expression:

$$\int_\Omega N_I \varepsilon(x_i,t)d\Omega = \int_\Omega N_I\left[\frac{\partial}{\partial x_i}\left(k_{ij}\frac{\partial h_{tr}}{\partial x_j}\right) - S\frac{\partial h_{tr}}{\partial t} - Q\right]d\Omega = 0 \tag{4.25}$$

where $\Omega$ represents the simulation region over which the integration (or summation) is performed. Using Green's 2nd identity, the spatial terms in equation (4.25) can be integrated by parts to yield the expression in equation (4.26) (after substituting for $h_{tr}$ using equation (4.23))

$$\int_\Omega k_{ij}\frac{\partial N_I}{\partial x_i}\frac{\partial N_J}{\partial x_j}d\Omega + \int_\Omega S N_I N_J \frac{\partial h_J}{\partial t}d\Omega + \int_\Omega N_I Q d\Omega - \int_B N_I\left(k_{ij}\frac{\partial h_{tr}}{\partial x_j}\right)n_i dB = 0 \tag{4.26}$$

where *B* represents the boundary of the simulation region. The integral expression representing the sink or source term in equation (4.26) may be evaluated using the expression:

$$Q = \sum_{I=1}^{n_w} q_I(x_{iI})\delta(x_i - x_{iI}) \tag{4.27}$$

where:

$q_I$ volumetric rate of injection/extraction per area at node $I$ [$L^1T^{-1}$],

$n_w$ number of wells, and

$\delta$ Dirac delta function.

Using equation (4.27) the integral expression representing the sink or source term $Q$, in equation (4.26) may be evaluated as:

$$\int_{\Omega} N_I Q d\Omega = q_I \tag{4.28}$$

The use of equation (4.27) implies that the right hand side of equation (4.28) is zero if node $I$ is not a sink or source node. The boundary integral expression in equation (4.26) may be evaluated by invoking the flux boundary condition defined for the flow governing equation, ie.,

$$-k_{ij}\frac{\partial h}{\partial x_j}n_i = q_n \tag{4.29}$$

Using equation (4.29) the flux boundary integral term in equation (4.26) becomes

$$-\int_B N_I\left(k_{ij}\frac{\partial h_{tr}}{\partial x_j}\right)n_i dB = \int_B N_I q_n dB \tag{4.30}$$

Incorporating equations (4.28) and (4.30) into (4.26), one obtains the following system of differential equations:

$$\int_{\Omega} k_{ij}\frac{\partial N_I}{\partial x_i}\frac{\partial N_J}{\partial x_j}h_J d\Omega + \int_{\Omega} S N_I N_J \frac{\partial h_J}{\partial t} d\Omega + q_I - \int_B N_I q_n dB = 0 \tag{4.31}$$

Equation (4.31) can be expressed in a more compact form as:

$$H_{IJ}h_J + P_{IJ}\frac{\partial h_J}{\partial t} = F_I \tag{4.32}$$

where:

$$H_{IJ} = \sum_e \int_{\Omega_e} k_{ij}\frac{\partial N_I}{\partial x_i}\frac{\partial N_J}{\partial x_j}d\Omega_e$$

$$P_{IJ} = \sum_e \int_{\Omega_e} SN_I N_J d\Omega_e$$

$$F_I = -\left(q_I + \sum_e \int_{B_e} N_I q_n dB\right)$$

$\Omega^e$ is the element subdomain with boundary $B^e$, $N_I$ and $h_J$ are interpolating functions and nodal values of head, respectively, and the summation is performed over the total number of elements. To complete the FEM formulation, a time integration is performed on equation (4.32) using the difference method. This procedure leads to the following system of algebraic equations:

$$\left(\theta H_{IJ} + \frac{P_{IJ}}{\Delta t_k}\right)h_J^{k+1} = \frac{P_{IJ}}{\Delta t_k}h_J^k + (\theta - 1)H_{IJ}h_J^k + F_I^{k+\theta} \tag{4.33}$$

where:

$k, k+1$ previous and current time levels, respectively, and

$\Delta t_k$ the $k$th time step.

$\theta$ is a time-weighting factor that lies between 0 and 1. In particular, $\theta$ = 1 leads to a fully implicit scheme while $\theta$ = 0.5 results in the Crank-Nicholson scheme which has the

advantage of a second order accuracy. Equation (4.33) is the final system of algebraic equations that must be solved to obtain the dependent variable $h_J$. The solution technique adopted to obtain $h_J$ is presented in section 4.4. The above formulation applies to both the two- and three-dimensional flow governing equations presented previously.

### 4.3.2 FEM Formulation of the 2-D Transport Model

Due to the occurances of high fluid velocities at some stages of the simulation process, there is the likelihood of solute transport being dominated by advection. It is known that the dominating character of the advective components of the transport model over their dispersive counterparts usually causes numerical dispersion [*Huyakorn and Nilkuha*, 1979; *Konikow and Bredehoeft*; 1978]. One common but expensive technique of overcoming numerical dispersion is the use of a sufficiently refined mesh. To alleviate this difficulty without the use of excessive refined mesh, *Huyakorn and Nilkuha* [1979] adopted the upstream-weighting function technique for one- and two-dimensional finite elements. This technique is used in the two-dimensional finite element formulation of the solute transport equation of the management model.

The upstream weighting function differs from the standard Galerkin technique by the fact that special weighting functions $W_I$ are used to *weight* the spatial terms in the advective-dispersive equation while the remaining terms are *weighted* by the usual interpolating functions $N_I$. To start the FEM formulation, let the domain be subdivided into a number of finite elements and let the trial solution to equation (4.22) $c_{tr}(x_i,t)$ , be approximated by the expression:

$$c_{tr}(x_i,t) = N_J(x_i)c_J(t), \quad i = 1,2, \quad J = 1,2,..,n \tag{4.34}$$

The upstream-weighting finite element procedure is executed by substituting the trial solution (equation 4.34) into equation (4.19) to generate the residuals. These residuals are forced to zero by weighting the spatial terms with the upstream-weighting function, $W_I$, and the remaining terms with the interpolating function $N_I$ and performing a summation (integration) over the entire simulation domain. Execution of these steps results in the following expression:

$$\int_\Omega W_I\left[\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c}{\partial x_j}\right)-v_i\frac{\partial c}{\partial x_i}\right]d\Omega-\int_\Omega N_I\left[R\frac{\partial c}{\partial t}+R\lambda c-\frac{Q_f}{m\theta}(c^*-c)\right]d\Omega=0 \qquad (4.35)$$

Application of Green's 2nd identity and substitution for $c_{tr}$ using equation (4.34) results in the following system of differential equations:

$$\begin{aligned}\int_\Omega\left[D_{ij}\frac{\partial W_I}{\partial x_i}\frac{\partial N_J}{\partial x_j}+v_iW_I\frac{\partial N_J}{\partial x_j}\right]c_J d\Omega+\int_\Omega N_IN_JR\frac{\partial c_J}{\partial t}d\Omega+\int_\Omega N_IN_J\left(\lambda R+\frac{Q_f}{m\phi}\right)c_J d\Omega \\ =\int_\Omega N_I\frac{Q_fc^*}{m\phi}d\Omega+\int_B W_I\left(D_{ij}\frac{\partial c_{tr}}{\partial x_j}n_i\right)dB\end{aligned} \qquad (4.36)$$

The boundary condition term in equation (4.36) can be evaluated directly using the specified flux equation (ie., equation (4.22)) of the transport model as follows:

$$\int_B W_I\left(D_{ij}\frac{\partial c_{tr}}{\partial x_j}\right)n_i dB=-\int_B W_Iq_f\left(c_{tr}+c_f\right)dB,\quad q_f=-v_in_i \qquad (4.37)$$

Substituting equation (4.37) into (4.36), a system of differential equations in a more compact form may be obtained as:

$$A_{IJ}c_J+E_{IJ}\frac{\partial c_J}{\partial t}=F_I \qquad (4.38)$$

where:

$$A_{IJ} = \sum_e \int_{\Omega_e} \left\{ \left( D_{ij} \frac{\partial W_I}{\partial x_i} \frac{\partial N_J}{\partial x_j} + v_i W_I \frac{\partial N_J}{\partial x_j} \right) + \int_{\Omega} N_I N_J \left( \lambda R + \frac{Q_f}{m\phi} \right) \right\} d\Omega$$

$$E_{IJ} = \sum_e \int_{\Omega_e} N_I N_J R d\Omega$$

$$F_I = \sum_e \left\{ \int_{\Omega^e} N_I \frac{Q_f c^*}{m\phi} d\Omega - \int_{B^e} W_I q_f (c_{tr} - c_f) dB \right\}$$

## 4.3.3 Upstream-Weighting Functions and Derivatives

For a typical rectangular element shown in Figure 4.1, the upstream-weighting function may be written in terms of the local isoparametric coordinates $(r,s)$ as in equations (4.39) to (4.42) [*Huyakorn and Nilkuha*, 1979]:

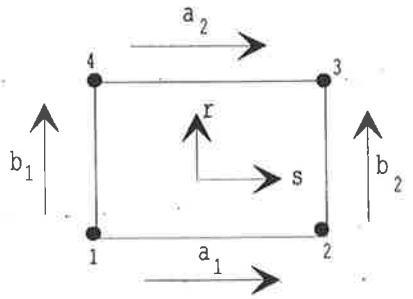



Figure 4.1 Quadrilateral element

$$-1 \le r \le 1$$
$$-1 \le s \le 1$$

$$W_1 = \frac{1}{16}\left[(1+s)(3a_1 s - 3a_1 - 2) + 4\right]\left[(1+r)(3b_2 r - 3b_2 - 2) + 4\right] \quad (4.39)$$

$$W_2 = \frac{1}{16}\left[(1+s)(-3a_1 s + 3a_1 + 2)\right]\left[(1+r)(3b_1 r - 3b_1 - 2) + 4\right] \quad (4.40)$$

$$W_3 = \frac{1}{16}\left[(1+s)(-3a_2 s + 3a_2 + 2)\right]\left[(1+r)(-3b_1 r + 3b_1 + 2)\right] \quad (4.41)$$

$$W_4 = \frac{1}{16}\left[(1+s)(3a_2 s - 3a_2 - 2) + 4\right]\left[(1+r)(-3b_2 r + 3b_2 + 2)\right] \tag{4.42}$$

where $a_1$, $b_1$, $a_2$, and $b_2$ are the upstream weighting factors associated with sides 1-2, 2-3, 4-3, and 1-4 of an element, respectively. For satisfactory results, *Huyakorn and Nilkuha* [1979] recommended that the derivatives of the upstream weighting functions must be evaluated in a manner that when differentiation is taken with respect to one particular coordinate, the value of the upstream parameters along the remaining coordinate must be set to zero, ie.,

$$\begin{aligned} \frac{\partial W_I}{\partial s}(a_i, b_j) &= \frac{\partial W_I}{\partial s}(a_i, 0) \\ \frac{\partial W_I}{\partial r}(a_i, b_j) &= \frac{\partial W_I}{\partial r}(0, b_j) \end{aligned} \tag{4.43}$$

For the typical element in Figure 4.1, the derivatives of the upstream-weighting functions may be expressed in terms of the local isoparameteric coordinates as follows [*Huyakorn and Nilkuha*, 1979]:

$$\frac{\partial W_1}{\partial s}(a_i, 0) = \frac{1}{4}(1-r)(3a_1 s - 1) \tag{4.44}$$

$$\frac{\partial W_2}{\partial s}(a_i, 0) = \frac{1}{4}(1-r)(3a_1 s - 1) \tag{4.45}$$

$$\frac{\partial W_3}{\partial s}(a_i, 0) = -\frac{1}{4}(1+r)(3a_2 s - 1) \tag{4.46}$$

$$\frac{\partial W_4}{\partial s}(a_i, 0) = \frac{1}{4}(1+r)\,(3a_2 s - 1) \tag{4.47}$$

$$\frac{\partial W_1}{\partial r}(0, b_j) = \frac{1}{4}(1-s)(3b_2 r - 1) \tag{4.48}$$

$$\frac{\partial W_2}{\partial r}(0, b_j) = \frac{1}{4}(1+s)(3b_1 r - 1) \tag{4.49}$$

$$\frac{\partial W_3}{\partial r}(0, b_j) = -\frac{1}{4}(1+s)(3b_1 r - 1) \tag{4.50}$$

$$\frac{\partial W_4}{\partial r}\left(0, b_j\right) = -\frac{1}{4}(1-s)(3b_2 r - 1) \tag{4.51}$$

Performing time integration on equation (4.38) using the difference method, the final system of algebraic equations to be solved may be obtained as:

$$\left(\theta A_{IJ} + \frac{E_{IJ}}{\Delta t_k}\right) c_J{}^{k+1} = (\theta - 1) A_{IJ} c_J{}^{k} + \frac{E_{IJ}}{\Delta t_k} c_J{}^{k} + F_I{}^{k+\theta} \tag{4.52}$$

The left-hand side matrix of equation (4.33) is symmetric while that of equation (4.52) is asymmetric. The asymmetric nature of equation (4.52) is the result of the advective component in the governing equations of the solute transport model. The appropriate solution techniques that conforms to each of these two sets of algebraic equations are presented in section 4.4.

### 4.3.4 FEM Formulation of the 3-D Transport Model

By substituting $W_I$ with $N_I$ and setting $i,j$ = 1,2 to $i,j$ = 1,2,3 , the finite element formulation of the three-dimensional transport model becomes identical to the procedures adopted for the two-dimensional Galerkin upstream-weighting technique. In fact, the only difference between the FEM formulation of the two- and three-dimensional solute transport models, is the use of the special upstream-weighting functions and derivatives in the two-dimensional scenario. Such upstream weighting functions and derivatives are not available in the three-dimensional case. Therefore replacing $W_I$ by $N_I$ and setting $i,j$ = 1,2 to $i,j$ = 1,2,3 reduces the two-dimensional formulation to the standard Galerkin finite element formulation in three-dimension; and the resulting system of asymmetric

algebraic equations are the same as in equation (4.52). The FEM formulation of the three-dimensional solute transport model is thus not repeated here.

## 4.4 Solution Techniques

The resulting system of algebraic equations to be solved for the flow and solute transport models are depicted in equations (4.33) and (4.52), respectively. The left hand side matrix of equation (4.33) is symmetric but that of equation (4.52) is asymmetric. In view of this a common solution technique is not applicable to both. However, an iterative solution technique can be used to solve the system of algebraic equations for both flow and solute transport without any modification. Three solution techniques : (1) Cheloski method for symmetric matrix (for the flow model), (2) Cheloski method for asymmetric matrix (for the transport model) and (3) a generalised iterative solver (applicable to both symmetric and asymmetric systems) are briefly presented.

### 4.4.1 Cheloski Method for Symmetric Matrix

Representing the left hand side matrix of equation (4.33) by $M$, the unknown head vector by $H$ and the right hand side vector by $B$ the resulting system of algebraic equations to be solved becomes:

$$[M]\{H\} = \{B\} \tag{4.53}$$

The Cheloski method is a direct method for solving a system of linear algebraic equations which makes use of the fact that $[M]$ can be decomposed into a product of an upper triangular matrix $[U]$, and its transpose, ie.,

$$[M] = [U]^T [U] \tag{4.54}$$

where the entries of $[U]$ are given by:

$$u_{ij} = \left( m_{ij} - \sum_{k=1}^{i-1} u_{ki}^2 \right)^{1/2}, \quad i = j \tag{4.55}$$

$$u_{ij} = \frac{m_{ij} - \sum_{k=1}^{i-1} u_{ki} u_{kj}}{u_{ii}}, \quad i < j \tag{4.56}$$

$$u_{ij} = 0, \quad i > j \tag{5.57}$$

where:

$u_{ij}$ = entries of $[U]$, and

$m_{ij}$ = entries of $[M]$.

Rewriting equation (4.53) as:

$$[U]^T [U]\{H\} = \{B\} \tag{4.58}$$

and defining a vector $\{Z\}$ as:

$$[U]\{H\} = \{Z\} \tag{4.59}$$

equation (4.58) can be expressed as:

$$[U]^T\{Z\} = \{B\} \tag{5.60}$$

from which the values in $\{Z\}$ can be obtained by the expression

$$z_i = \frac{\left(b_i - \sum_{k=1}^{i-1} u_{ki} z_k\right)}{u_{ii}}, \quad i = 1,2..,n \tag{4.61}$$

where:

$b_i$ = entries of $\{B\}$,

$z_i$ = entries of $\{Z\}$, and

$n$ = number of unknown nodes in the finite element network.

Once the entries of $\{Z\}$ have been evaluated, the entries of $\{H\}$ (the nodal hydraulic heads) are obtained from equation (4.59) using the expression:

$$h_{n+1-i} = \frac{\left(z_{n+1-i} - \sum_{k=1}^{i-1} u_{n+1,n+1-k} h_{n+1-k}\right)}{u_{n+1-i,n+1-i}}$$

## 4.4.2 Cheloski Method for Asymmetric Matrix

The Cheloski method as an asymmetric solver makes use of the fact that any square matrix [$M$], as in equation (4.53) can be expressed as the product of a lower triangular matrix [$L$] and an upper triangular matrix [$U$], ie. ,

$$[M] = [L][U] \tag{4.62}$$

$M$ is said to have been decomposed or factored into the product of two triangular matrices and this step of the Cheloski method is sometimes referred to as the triangular decomposition of $[M]$. The entries of $[L]$ and $[U]$ are given by:

$$l_{ij} = m_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj}, \qquad i \geq j \tag{4.63}$$

$$l_{ij} = 0 \qquad i < j \tag{4.64}$$

$$u_{ij} = \frac{m_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}}{l_{ii}}, \qquad i < j \tag{4.65}$$

$$u_{ij} = 1, \qquad i = j \tag{4.66}$$

$$u_{ij} = 0, \qquad i > j \tag{4.67}$$

where:

$l_{ij}$ = entries of $[L]$

Equation (4.53) can now be expressed as

$$[L]\,[U]\,\{C\} = \{B\} \tag{4.68}$$

where:

$\{C\}$ = vector containing unknown concentration values

If a vector $\{Z\}$ is defined as:

$$[U]\{C\} = \{Z\} \tag{4.69}$$

then equation (4.68) may be written as:

$$[L]\{Z\} = \{B\} \tag{4.70}$$

from which the values of $\{Z\}$ , $z_i$, may be obtained as:

$$z_i = \frac{\left(b_i - \sum_{k=1}^{i-1} l_{ik} z_k\right)}{l_{ii}}, \qquad i = 1,2,\ldots n \tag{4.71}$$

With the values of $\{Z\}$ computed, the concentration values (the entries of $\{C\}$ ) can now be obtained through a backward substitution step in equation (4.69) as:

$$c_{n+1-i} = z_{n+1-i} - \sum_{k=1}^{i-1} u_{n+1-i,n+1-k} c_{n+1-k} \tag{4.72}$$

### 4.4.3 Gauss-Siedel Iteration

Even with the storage savings in direct solution methods presnted above, the storage requirements are still large for problems of large finite element network. Therefore the use of iterative methods have become very important in groundwater

modelling since they generally need much less storage space, solves the problems faster, and are applicable to both symmetric and asymmetric solvers without modifications. Because of the considerable number of times that the objective function (and hence the forward problem) is evaluated in the inverse analysis, a much faster method of solving the system of equations is required. Hence, the use of the Gauss-Siedel method in the inverse problem of parameter identification.

The theory of the method can be found in many text books on numerical analysis [eg. *Carnahan et al.*, 1969]. The system of linear equations is written as:

$$\sum_{I,J=1}^{N} \{P(I,J) * F(J)\} = G(I) \tag{4.73}$$

where $N$ is the number of nodes in the finite element network, $P$ may be a symmetric or asymmetric matrix, $F$ may be a vector of unknown heads or concentration values, and $G$ is the right hand side load vector. In the Gauss-Siedel method, an initial estimated solution is continuously updated by correcting the I*th* equation by modifying variable $I$. The initial estimate may be arbitrary, for example $F(I) = 0$ for all unknown values of $F(I)$. Alternatively one may make some reasonable guess for the unknown variable. In general equation (4.73) will not be satisfied by the estimated solution on substitution of the initial guesses. The variable $F(I)$ is now corrected, by an amount $DF(I)$, such that equation $I$ is satisfied. If the estimated solution is denoted by $FA(I)$, it means that

$$\sum_{I,J=1}^{N} \{P(I,J) * FA(J) + P(I,I) * DF(I)\} = G(I) \tag{4.74}$$

From equation (4.74), the unknown correction $DF(I)$ can be determined from the equation:

$$DF(I) = \frac{\left[ G(I) - \sum_{I,J=1}^{N} \{ P(I,J) * FA(J) \} \right]}{P(I,I)} \qquad (4.75)$$

The Gauss-Siedel algorithm now consists of a repeated execution of equation (4.75) for all values of *I*. That the process must be repeated follows from the fact that, by application of equation (4.75), the *Ith* equation is satisfied, but this is distributed later by updating other values. It can be shown that the Gauss-Siedel procedure converges, provided that the matrix *P* is *positive-definite*. Convergence is reasonable fast if the main diagonal of the matrix is dominant. Rate of convergence is further improved by multiplying the correction in each updating step by the so-called *over-relaxation factor R*. *R* lies between 1 and 2. If *R* is chosen too large (ie., $R > 2$), the iterative scheme will diverge.

In many physical applications, a large proportion of the elements of matrix *P* are zero , which means that a considerable amount of computer memory and computation time is wasted by storing zeros, and by multiplications by zero. In fact it can be expected that only a few elements of *P* are different from zero. This property can be used to save computer time and memory by separate storage of the precise locations of the nonzero coefficients in *P* through the use of the concept of *pointer length* and *pointer matrix*. Details of this concept can be found in *Kinzelbach* [1986]. The entire flow chart for the finite element analysis of either flow or solute transport with direct solution techniques is shown in Figure 4.2. In the inverse analysis, the two solvers in Figure 4.2 are replaced with a generalised iterative solver which uses the concept of pointer length and pointer matrix.

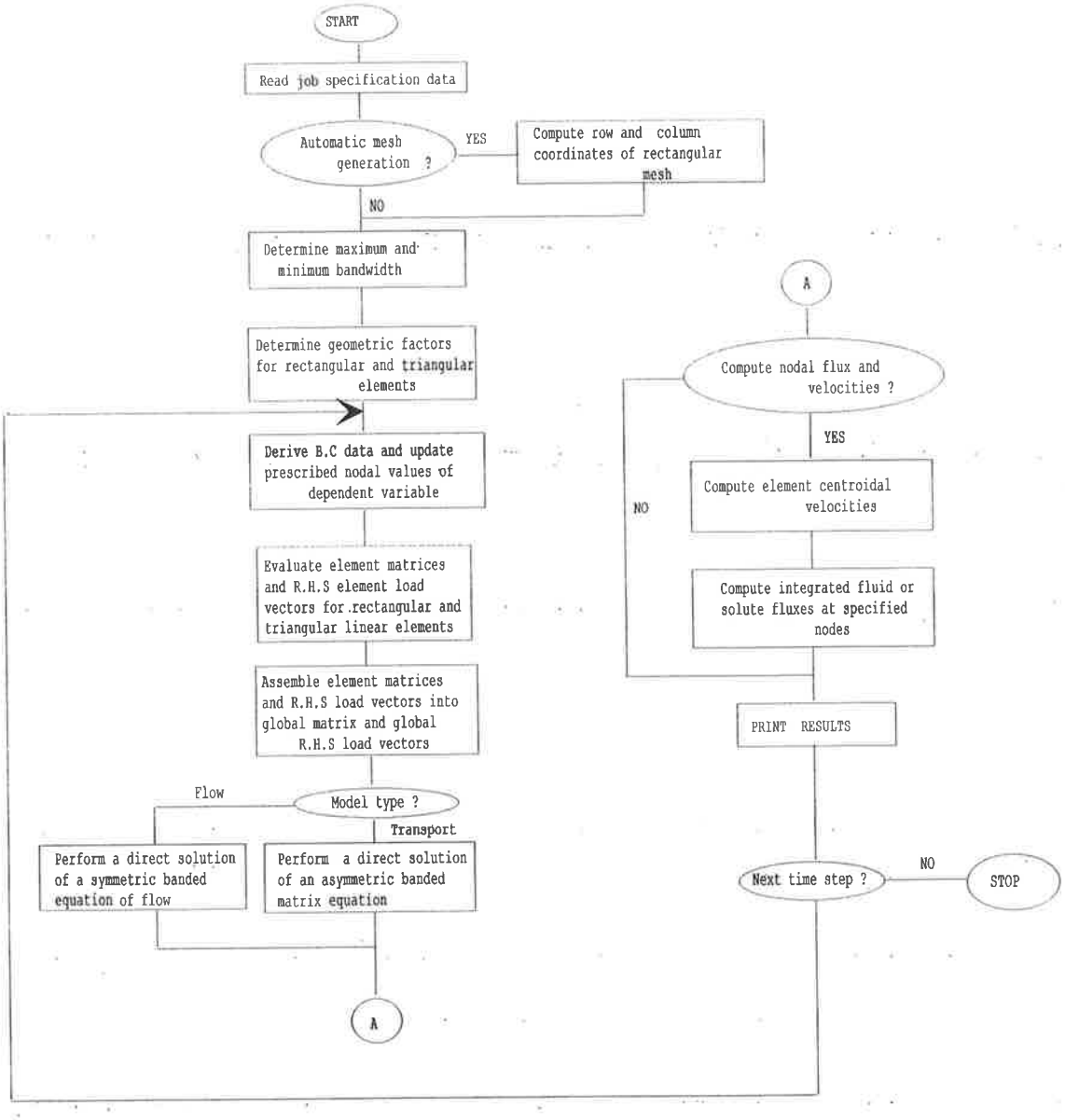



**Figure 4.2** Schematic representation of the analysis of flow or solute transport.

# 4.5 Summary

This chapter has presented the governing equations, the finite element formulation and solution techniques to be employed in the two evolutionary optimisation techniques

proposed in this research work. The governing equations involve the flow and solute transport models in both two- and three-dimensional systems. These governing equations are reduced to a system of solvable algebraic equations using the finite element formulation technique. The solution techniques for system of algebraic equations have been presented using the Cheloski method for symmetric matrices (for the flow model) and Cheloski method for asymmetric matrices (for the solute transport model) and a generalised iterative solver applicable to both symmetric and asymmetric systems. These models are eventually interfaced with the evolutionary optimisation techniques presented in chapter five.

# Chapter 5

# Optimisation Techniques

## 5.1 Introduction

The parameter estimation and the remediation design (or contaminant extraction) processes are both pursued via optimisation techniques. The genetic algorithm and the shuffled complex techniques are all evolutionary optimisation processes that are to adopted in the remediation design and the parameter estimation models, respectively. This chapter presents the following (1) a brief introduction to genetic algorithm, (2) formulation of the genetic algorithm with respect to remediation design, and (3) presentation of the shuffled complex evolution (SCE) and its formulation for the inverse problem of parameter identification.

## 5.2 Genetic Algorithm - Introduction

This introductory section on genetic algorithm (GA) is based on the realisation of *Ritzel et al.* [1994]. These authors define GA as a search technique that is designed to mimic some of the most salient features of natural selection and natural genetics in order to find the near-optimal solution in a search space. According to these workers, the GA has the capability to search complex multimodal decision spaces and can efficiently handle nonconvexities that cause difficulties for traditional gradient-based optimisation methods. As stated by *Goldberg* [1989], the structure of genetic algorithm differs from the more

traditional gradient-based methods in four major ways : (1) the genetic algorithm typically uses a coding of the decision variable set , not the decision variables themselves; (2) the genetic algorithm searches from a population of decision variable sets, not a single variable set; (3) the genetic algorithm uses the objective function itself , not derivative information; and (4) the genetic algorithm uses probabilistic, not deterministic, search rules.

A GA operates on a *population* of decision variable sets. These decision variable sets are called *strings*, or by an analogy to biological model, *chromosomes*. Each string is made up of a series of *characters*, or analogous to biology, *genes*. The characters represent a coding of the decision variable set. The coding can be binary, integer or real. However, *Goldberg* [1989, pp. 80-82] has suggested that the performance of a GA is optimal when a binary coding is implemented, although construction with real or integer numbers is more directly representative of the actual decision variables. The genetic coding of a string is called its *genotype* while the decoded decision variable set is referred as the string's *phenotype*. The values of the genes are chosen initially at random. The number of strings in a GA operation may vary but it is typically within the range 30-100 [Goldberg, 1989]. After a population of strings are initialised, the optimisation operates through a repeated evaluation of four major genetic operators : (1) selection, (2) mutation, (3) crossover, and (4) inversion. The GA terminologies string, parent, and chromosome are used to represent decision variables in the optimisation process. Therefore unless otherwise stated, they may be used interchangeably to represent the same phenomenon.

### 5.2.1 Selection

This procedure is implemented to select the appropriate strings or parents for reproduction. The selection procedure is based on comparison of *fitnesses*. To determine fitness, each string's is first decoded into the decision variables. These are then used to determine the value of the objective function. The objective function value is usually used to represent the string's fitness. The mechanism relating a string's fitness to its probability of selection is a subject of considerable research. *Goldberg* [1989] has presented several selection techniques. Among these, the binary tournament selection is the most popular. The binary tournament selection begins by picking two strings at random and comparing their fitnesses. The string with a better fittness wins the tournament and enters a temporary mating pool to await mating. The binary tournament selection is repeated until a mating pool, as large as the original population is generated.

A more generalised selection procedure is the *s-member tournament* selection which involve the selection of $s$ (where $s$ represents a number parents participating in the competition and lies in the between 2 and the population size) parents for the impending crossover operation. The fitness of each parent is obtained as explained previously. Parents with better fittnesses are transferred into a pool of eligibles to await mating. The number of victors or winners , *nwin* , from the randomly selected $s$ parents, who find their way into the mating pool range between 1 and $s$, inclusive. The $s$-member tournament selection process is repeated until the expected number of the population of parents in the mating pool is achieved. For the remediation problem, the simplest case of tournament selection ($s$ = 2 and *nwin* = 1) is employed. This involves two parents competing against each other with one winner entering the mating pool.

### 5.2.2 Crossover

The mating pool represents the population of parents that survive to create a new generation. Children are created in a process known as crossover. A simple crossover operation begins by selection of two strings from the mating pool. A crossover site is randomly selected for the two strings. Then the genetic material after the crossover site is exchanged between the two selected strings. The two new strings formed are considered *children* and they form members of the new generation. The genetic operation of crossover is performed on each mated pair with a certain probability referred to as the probability of crossover, *p_cross*. In most analysis, the probability of crossover is set so that the crossover operation is performed on most, but not all, of the population. The end result of the crossover operation is the creation of a new population consisting of children strings whose parents no longer exist and a minority of the parents who are lucky enough to enter the new population unaltered. This new population of children form the parents of the next generation.

In summary, crossover permits parents in the mating pool to form the children (who become the parents in the next generation). It is considered as the central feature in GAs. It results in different varieties of decision variables and hence ensures that each child in the new population is unique and thus has the capability of generating a unique objective function value (the measure of the fitness of a parent or chromosome). In a more generalised crossover operation, a randomly selected number of parents (*n_par*) from the mating pool who have not yet participated in the mating exercise is first made. In this case *n_par* is usually greater than 2. Comparing a generated random number to the probability of crossover *p_cross*, a change in genetic material of the *n_par* parents selected is executed in a cyclic fashion at a number of randomly selected crossover sites (*n_site*), if the generated random number is less than or equal to *p_cross*. The value of *n_site* must range between 1 and the total number of genes (*n_genes*) on a parent. A generalised crossover event with

*n_par* = 4, *n_genes* = 10 and *n_site* = 2, is shown in Figure 5.1. This illustration assumes that the randomly selected sites are after the 4th and 9th gene locations. The simplest case of crossover operation (point crossover) is achieved when *n_par* = 2, and *n_site* = 1. The point crossover operation is illustrated in Figure 5.2 where it is assumed that the crossover site is randomly selected after the 5th gene.

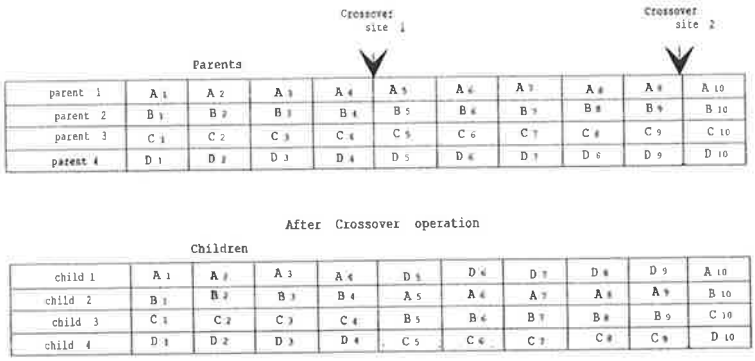



**Figure 5.1** Representation of a cyclic crossover operation

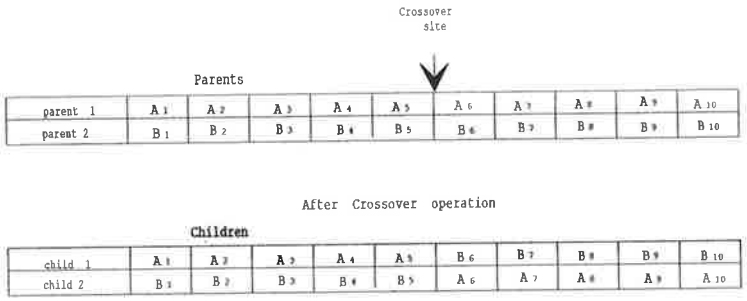



**Figure 5.2** Representation of point crossover operation

For *n_site* = *n_gene* - 1, a uniform crossover operation is executed. If the generated random number is greater than *p_cross*, the crossover operation is omitted. In the design of the proposed remedial optimisation program the simplest (or point) crossover operation is employed.

### 5.2.3 Mutation

Mutation is a single chromosome operation that is employed to alter the binary bit (gene) value on the children reproduced from crossover. Mutation of genes introduces diversity into the new generation which in turn reduces the possibility of premature convergence of the optimisation operation onto a local optimum. In the mutation operation, a random number is first generated for the chromosome in question and compared to a value called the probability of mutation, *p_mute*. If the generated random number is less than *p_mute*, the mutation operation is executed otherwise it is omitted. If mutation must be executed, a binary bit on the chromosome is randomly selected and its value is changed from 0 to 1 and vice versa.

### 5.2.4 Inversion

Similar to the mutation operator, inversion is a single chromosome operation that reverses the order of the binary bits within two randomly selected locations based on a decision value called the probability of inversion, *p_invrs*. For inversion to occur, the value of a generated random number must be less than or equal to *p_invrs*. The inversion operation begins by the random selection of two locations along the chromosome in question. The binary bits within the selected locations are subsequently reversed. The objective of inversion is to introduce unique chromosomes and hence prevent the formation of species of the same kind. *Goldberg* [1989] has mentioned that formation of species of the same kind tend to produce low performance offsprings (which he calls lethals). The process of inversion is illustrated in Figure 5.3 with a randomly selected locations after the 4th and 9th genes for a chromosome with *n_genes* = 10.

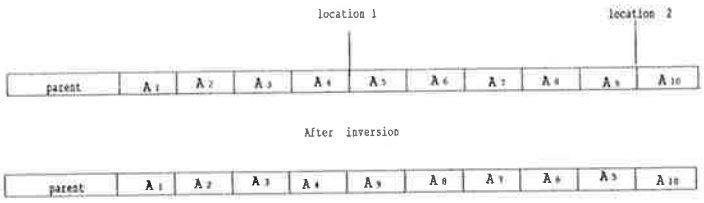



**Figure 5.3** Representation of single-chromosome inversion

### 5.2.5 How the GA Works

Every optimisation model requires a function to optimise. Such functions are usually called the objective (or criterion) function. Depending on the nature of the problem, the objective function may be a complex management decision model with a given number of parameters and constraints. In conceptual rainfall runoff calibration or aquifer parameter estimation, the objective function may usually be expressed as a standard least squared type. The work of the GA is the repeated evaluation of the objective function till a certain convergence criterion is met. This involves the automatic variation of the decision variables through the execution of the four genetic operators described previously. In a population comprising $m$ parents for example, the objective function is evaluated $m$ times (using the decoded value of each string), resulting in $m$ unique children (who become parents in the next generation). The objective function value for each parent become the fitness in GA context, which is subsequently used in the tournament selection procedures.

The new parameters (or decision variables) for each generation are obtained through the four genetic steps of selection, crossover, mutation, and inversion using the previous computed values of their fitnesses. The entire communication between the GA and the objective function is the passage of fitness values corresponding to each parent from the from the objective function to the GA, or the passage of decoded parameter values from the GA to the objective function. This back and forth passage of information may go on for a certain number of generations or until a convergence criterion is met. At the end of each

generation the best values of the objective function is saved. This allows the comparison of $n$ (where $n$ is the number of generation set for a given problem) best values from which the optimum best solution is selected. The next section illustrates how the GA is formulated to solve a specific problem - the proposed optimisation model for contaminant extraction.

## 5.2 Application of GA to a Remediation Scheme

The genetic operators presented in the previous sections are the standard steps in any optimisation program based on GAs. In fact, for any specific optimisation scheme, the GA technique will have to be formulated to suite the purpose of the scheme in order to yield the desired results. In remediation scheme, the most important steps are the representation of the decision variables and their incorporation into the objective function. The objectives are: (1) how many extraction wells to install, (2) where to install them, (3) pumping rate of each extraction well, and (4) the cost of the entire installation and extraction operation. The remediation scheme requires the optimisation of all these objectives.

### 5.2.1 Representation of Decision Variables

The present program is designed in a manner that allows all the parameters under optimisation to be determined simultaneously at the end of each run. In view of this, the decision variables (extraction wells) are represented as binary bits on each string. To present four possible pumping rates at each well for the GA to optimise from, two binary bits are used to represent the status of each extraction well. Since a binary bit can be 1 or 0, each extraction well can have 4 ($2^2$) possible pumping rates. The status of seven extraction wells, for instance, is shown in Figure 5.4. Each of these wells may have four possible

pumping rate options. If at the start of a remedial scheme, pumping rates of $25\,m^3d^{-1}$ and $50\,m^3d^{-1}$ are allocated to each binary bit location, then the four possible pumping options may be :

**0 0** = inactive ( or $0\,m^3d^{-1}$ )

**0 1** = $25\,m^3d^{-1}$

**1 0** = $50\,m^3d^{-1}$

**1 1** = $75\,m^3d^{-1}$

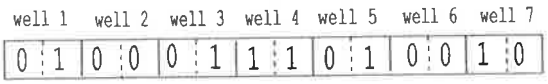



**Figure 5.4** Representation of wells as decision variables along a string

This coding configuration is applied to all extraction wells represented by binary bits along the entire length of the population of strings. The use of the scheme shown in Figure 5.4 indicates that the status of a string (hence extraction wells) will remain constant in the entire time step of the numerical model, once this string is in use. The location of contaminant plumes however, varies throughout the time span of the embedded numerical forward model. Therefore the use of Figure 5.4 may render some of the extraction wells redundant as the contaminant plume moves with time. To account for this redundancy, a time-variation scheme is incorporated as an alternative to the coding configuration shown Figure 5.4. The time-variation scheme is shown in Figure 5.5. In this scheme, the number of simulation time steps set for the numerical model is partitioned into distinct sub-time interval and a string allocated to each sub-time interval. In this research study, only three sub-time intervals $T_1$, $T_2$, and $T_3$ are used. This particular number of sub-time interval has been selected to match the available computer memory resources. On large machines one

can consider the use of more than three sub-time steps. If $T$ is the entire number of time steps set for the numerical model, then $T = T_1 + T_2 + T_3$.

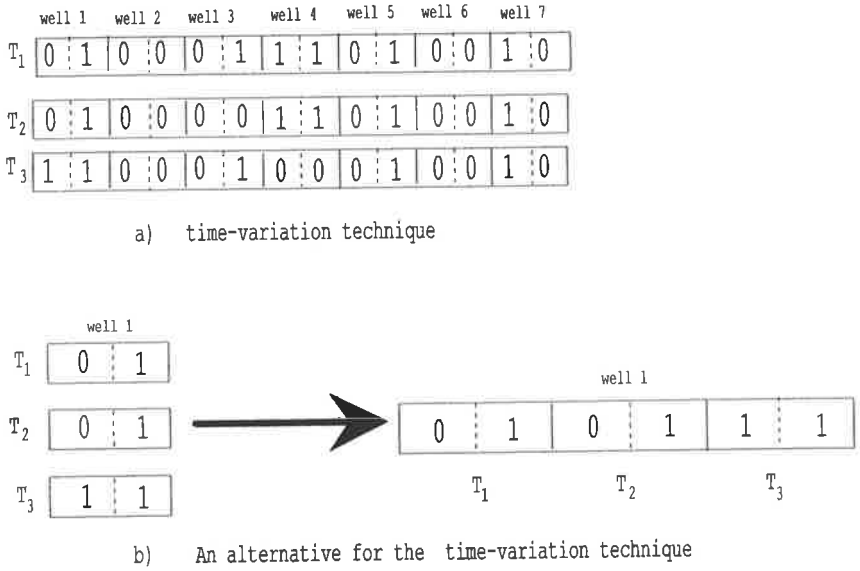



**Figure 5.5** Representation of wells in the time-variation scheme.

After initialisation of the population of parents (or strings), the time-variation scheme follows the basic four genetic operators: (a) selection, (b) crossover, (c) mutation, and (d) inversion. The crossover operation for the time-variation and non time-variation coding configuration are shown in Figure 5.6. The next section addresses the objective function which is referred to as the cost function in this research study.

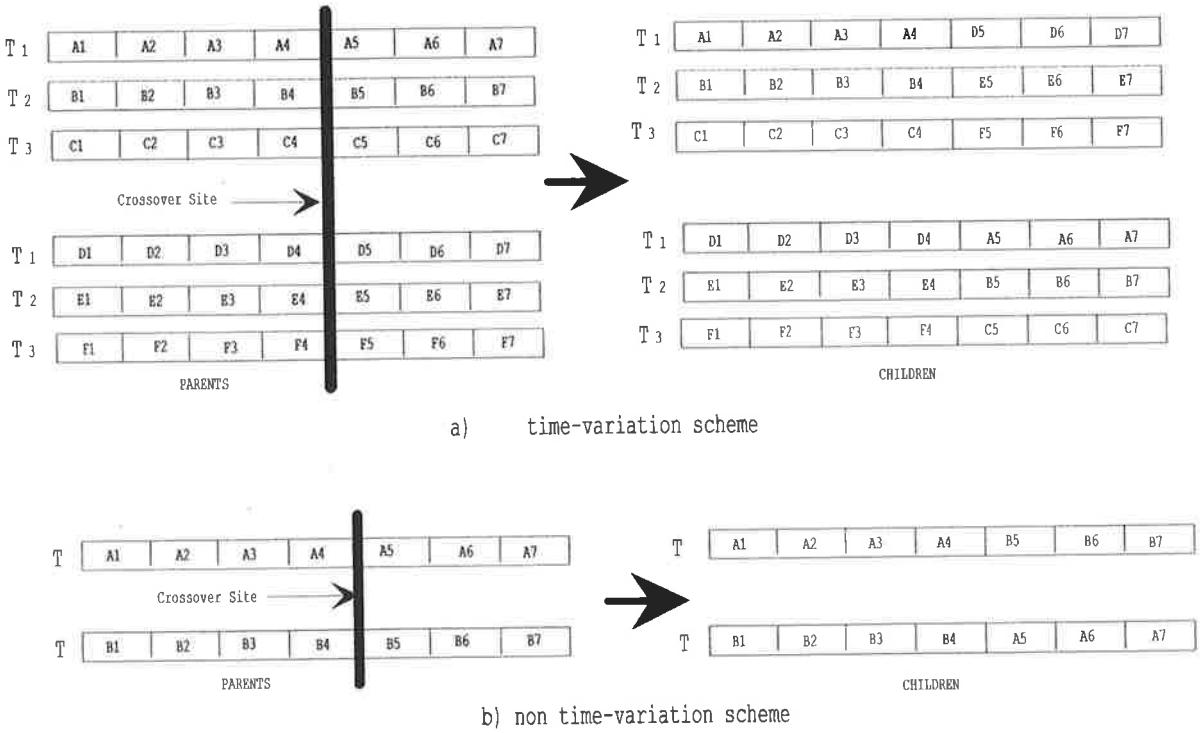



**Figure 5.6** Schematic representation of a cross over operation

## 5.2.2 Cost Function for the Remediation Scheme

The optimum design for the remedial action is the most economic method of reducing the concentration of the pollutant to acceptable levels. This requires the following factors to be considered: (1) number of extraction wells to be installed, (2) the location of the extraction wells, (3) rate of pumping at each well , (4) period of pumping, and (5) treatment of the polluted water. The cost associated with the setting up of each well, and the pumping and treatment cost are lumped together in two parameters namely: (a) the initial cost of setting up the well, and (b) the cost per unit volume of pollutant extracted. Several options exist to reclaim or control a contaminated aquifer. These include in-situ bioremediation, slurry walls, pump-and-treat etc. The pump-and-treat is relatively inexpensive and accommodates all types of pollutants, whether biodegradable or not. It is

therefore assumed that the pump-and-treat strategy is adopted, and that the method of treatment has already been determined. Furthermore, it is assumed that the physical and hydraulic properties for both flow and solute transport are known with certainty. The cost to be optimised $c_{op}$, for the entire extraction operation is expressed as:

$$c_{op}(w_1, w_2, .., w_{n_{ew}}) = An_{ew} + Bv_{tr} + \sum_{i=1}^{nn} p_n(c - c_{ut}) + pv \qquad (5.1)$$

where:

| | |
|---|---|
| $A$ | initial cost per well installed [$] |
| $B$ | cost of treatment per volume of water extracted [$], |
| $v_{tr}$ | volume of fluid treated [$L^3$], |
| $n_{ew}$ | number of extraction wells installed, |
| $nn$ | number of nodes in the discretized simulation domain, |
| $c$ | nodal concentration at time $t$ [$ML^{-3}$] |
| $c_{ut}$ | permitted concentration level in the simulation domain [$ML^{-3}$], |
| $w_i$ | extraction well $i$, |
| $p_n$ | nodal penalty factor if $c > c_{ut}$ [$], and |
| $pv$ | global penalty value [$] if $c > c_{ut}$ anywhere |

The values of $c$ at the right hand side of equation (5.1), the nodal concentration in the simulation region at any time level of the extraction operation. These values are obtained from the numerical transport model already presented and formulated in chapter four.

### 5.2.3 Penalty

Because of the possibility that concentration levels evaluated during extraction may exceed the permitted concentration level ($c_{ut}$) within the aquifer, it is necessary to impose penalties for sensible determination of the fitness of each string. To differentiate between trial solutions with the same number of pumps and volumes extracted, a penalty function which is proportional to the concentration excess over the permitted concentration ($c_{ut}$) is imposed at each node. In an event where $c \leq c_{ut}$ (where $c$ the concentration of a node at any time $t$), the nodal penalty function is zero. A further penalty value of $pv$ is imposed if at any node the concentration is above $c_{ut}$ at the end of the simulation time. In this regard, the penalty value is zero if the concentration levels everywhere within the simulation region is below $c_{ut}$ at the end of the simulation time. This is to ensure that a solution that has unacceptable contaminant levels is not more acceptable, from cost considerations, than a solution that reduces the contaminant levels to below the maximum acceptable levels but at a greater cost. Imposing penalties for violation of the permitted concentration prescribed by management is analogous to the use of constraints in traditional gradient-based optimisation problems. A flow chart showing the remedial clean up operation is shown in Figure 5.7.

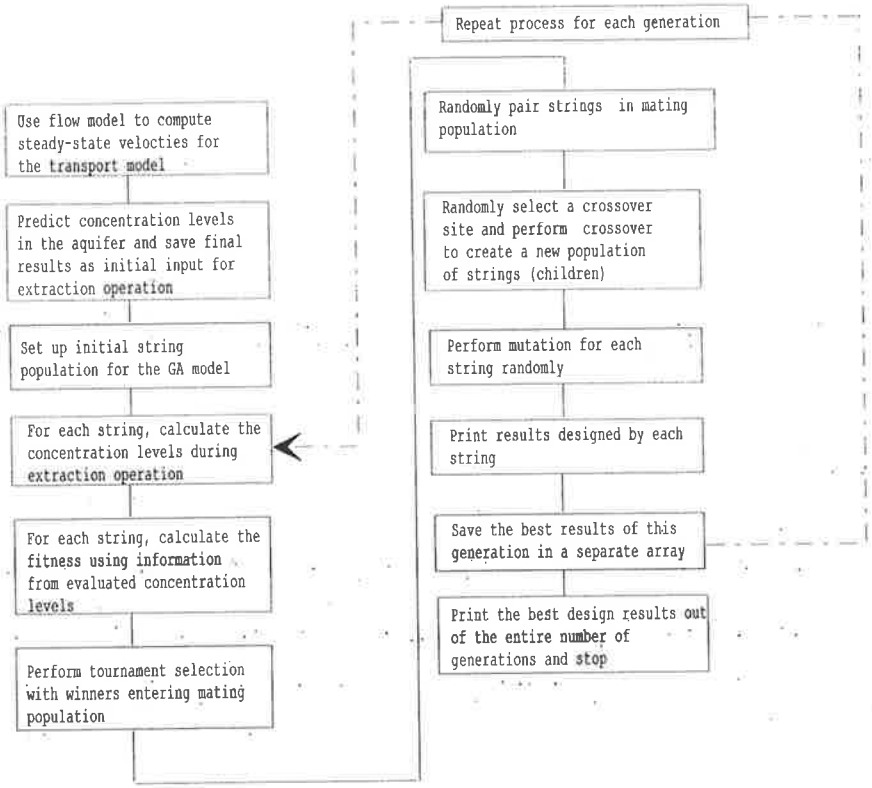



**Figure 5.7** Flow chart of a remediation scheme

## 5.3 Parameter Estimation (Inverse Problem)

To build a model for real groundwater system, two problems, the forward problem (simulation) and its inverse (calibration), must be solved. The former predicts unknown system states by solving appropriate governing equations (as presented and formulated in chapter four), while the latter determines unknown physical parameters and other conditions of the system by fitting observed system states.

The progress of the inverse solution techniques have been hampered by several inherent difficulties. First, the inverse problem is often ill-posed (ie., its solution may be non-unique and unstable with respect to observation error). Secondly the quality and quantity of observation data are usually insufficient. Thirdly, the model structure error, which is difficult to estimate, often dominates other errors. Therefore to obtain reliable

results at all costs, a more robust, efficient, and effective search technique is required to handle these problems. For the past three decades various forms of the gradient-based techniques have been used to handle groundwater inverse problems. Although some considerable amount of success have been reported, the problems of ill-conditioning (singularity of the normal matrix) and instability of parameters under estimation (as a result of data quality and quantity) have not yet been resolved.

Recently, a study by *Duan et al.* [1992] on a six parameter model using synthetic data uncovered five major problems that characterise the major solution difficulties of calibration processes: (1) the presence of several regions of attraction into which a search strategy may converge, (2) presence of numerous local minima in each major region of attraction, (3) non-smoothness and discontinuous nature of the objective function in the multiparameter space (with possible discontinuous derivatives which may vary in an unpredictable manner through the parameter search space), (4) exhibition of varying degrees of sensitivities by the parameters of the model under consideration, and (5) nonlinearity of the solution response surface near the true solution.

An optimisation algorithm that deals with the above mentioned problems must possess the following qualities [*Duan et al.*, 1994]: (a) ability to converge globally in the presence of multiple regions of attraction, (b) ability to avoid being trapped by 'pits' and 'bumps' over the objective function surface, (c) must be robust in the presence of differing parameter sensitivities and parameter interdependencies, and (d) must possess the power to handle a model with high parameter dimensionality. With all these qualities embedded in the shuffled complex evolution (SCE) optimisation technique, it has been selected as the best technique to be adopted in the present research study for solving the inverse (or parameter estimation ) problem proposed in this research study.

The SCE methodology was developed by *Duan et al.* [1992,1993] at the University of Arizona for the calibration of difficult and complex conceptual rainfall runoff (CRR) models. The literature survey has indicated that the technique has never been extended in

the history of groundwater modelling to solve the inverse problem of parameter identification. It is based on four concepts namely: (i) combination of deterministic and probabilistic concepts, (ii) systematic evolution of a complex of points spanning the parameter space in the direction of global improvement, (iii) competitive evolution, and (iv) complex shuffling. The synthesis of these four concepts make the SCE algorithm not only effective and robust but also flexible and efficient. The use of deterministic strategies permit the SCE algorithm to make effective use of the response surface information to guide the search. Robustness and flexibility is taken care of by the use of random elements. Concentrating a search in the most promising region of the search space is guided by the implicit clustering strategy. The use of systematic complex evolution strategy helps to ensure a relatively robust search that is guided by the structure of the objective function. The entire optimisation algorithm comprises two procedures : (a) the shuffling of complexes and (b) the competitive complex evolution (responsible for the generation of offsprings).

### 5.3.1 SCE Algorithm

The SCE method combines the strengths of the simplex procedure of *Nelder and Mead* [1965] with : (i) the concept of controlled random search [*Price*, 1987]; (ii) competitive evolution [*Holland*, 1975]; and (iii) the concepts of complex shuffling [*Duan et al.*, 1992, 1993]. Essentially the method begins with a population of points sampled randomly from the feasible region. The population is partitioned into communities (or complexes), each of which is allowed to evolve (generate offsprings) independently on the basis of a statistical reproduction process that employs the complex geometric shape to direct the search in a refined direction. In the course of the evolutionary process, the entire population is shuffled and points are reassigned to complex or communities to allow for sharing of information from the individual communities. A continuous repetition of this

process forces the population to converge towards the neighbourhood of the global optimum if the initial size of the population is sufficiently large [*Duan et al.*, 1994]. From the realisation of *Duan et al.* [1992,1993], the SCE algorithm is enumerated below and its flow chart is shown schematically in Figure 5.8. The use of the term *function* in the algorithm below typically refers to the objective function posed in equation (5.4).

**1)** Initialise the number of complexes $p$ and the number of points in each complex $m$. Compute the sample size $s$ as $s = pm$.

**2)** Generate a sample of $x$ points $x_1, x_2, \ldots, x_s$ in the feasible space $\Omega \subset \Re^n$ and compute the function value $f_i$ at each point $x_i$; using uniform sampling distribution in the absence of prior information.

**3)** Sort the $s$ points in order of increasing function value and store them in array $D = \{x_i, f_i, i = 1,2,\ldots,s\}$ such that $i = 1$ represents the function with the smallest function value.

**4)** Partition $D$ into $p$ complexes $A^1, A^2, \ldots, A^p$, each containing $m$ points, such that $A^k = \left\{x_j^k, f_j^k \middle| x_j^k = x_{k+p(j-1)}, f_j^k = f_{k+p(j-1)}, j = 1,\ldots,m\right\}$.

**5)** Evolve each complex $A^k, k = 1,\ldots,p$ using the competitive complex evolution (CCE) algorithm described in section 5.3.2.

**6)** Shuffle the complexes by replacing $A^1,\ldots,A^p$ into $D$ such that $D = \{A^k, k = 1,\ldots,p\}$ and sort $D$ in order of increasing function value.

**7)** Check for convergence. If convergence criteria are satisfied, stop; otherwise continue.

**8)** Check the reduction in the number of complexes - if the minimum number of complexes required in the population , $p_{min}$, is less than $p$, remove the complex with the lowest ranked points; set $p = p - 1$ and $s = pm$ and return to step 4. If $p_{min} = p$ return to step 4 without reducing the size of $p$.

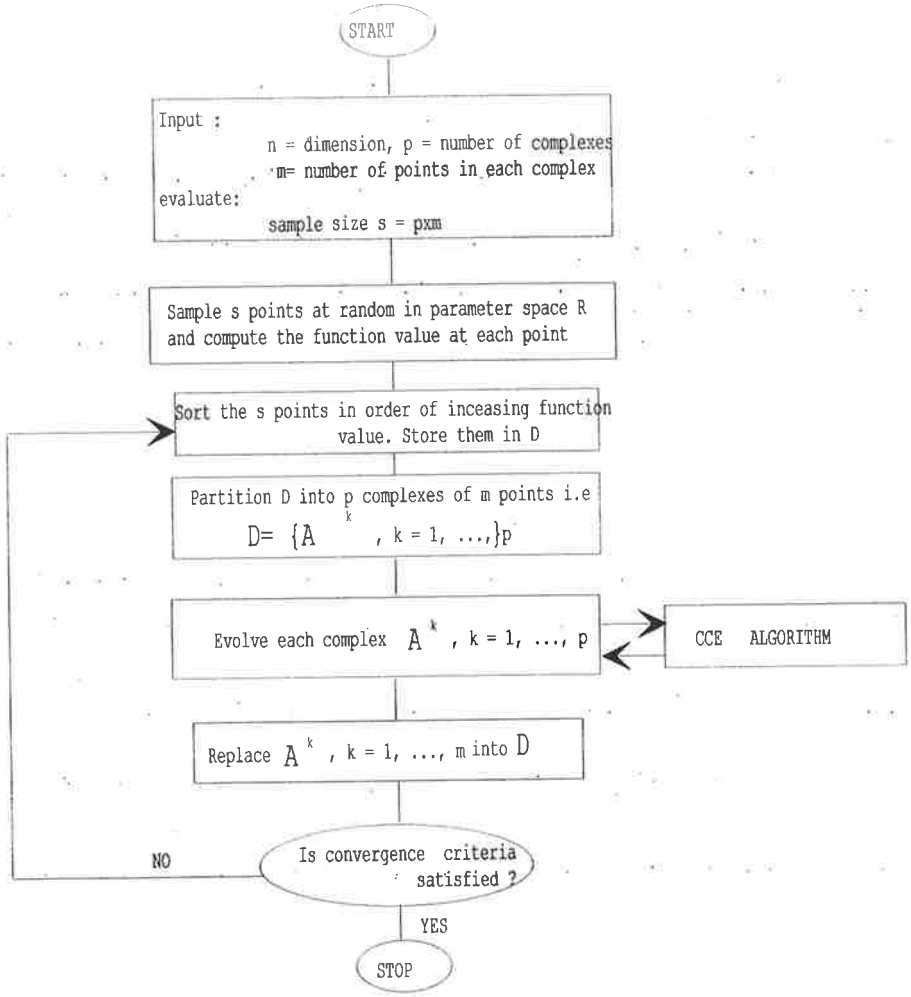



**Figure 5.8** Schematic representation of the SCE algorithm

### 5.3.2 CCE Algorithm

The CCE algorithm is the major component of the shuffled complex evolution methodology. It employs the Simplex downhill search method of *Nelder and Mead* [1965] in the generation of offsprings. This scheme is not sensitive to nonsmoothness of the response surface. This property of the Simplex scheme allows the entire SCE algorithm to take full advantage of the response surface information to guide the search towards an improved direction. The algorithm is presented below from the realisation of *Duan et al.*, [1992, 1993] where the object is to minimise the objective function. A schematic representation of the flow of the CCE algorithm is shown in Figure 5.9.

**1)** Select $q$, $\omega$ and $\beta$; where $q$ is the number of subcomplexes , $\omega$ is the expected number of times that an offspring is generated, and $\beta$ is the number of times each complex is expected to evolve.

**2)** Assign a triangular probability distribution $\rho_i$ to $A^k$ using the expression

$$\rho_i = \frac{2(m+1-i)}{m(m+1)}, \qquad i = 1,\ldots,m \tag{5.2}$$

where the point $x_1{}^k$ has the highest probability of $\rho_1 = 2/(m+1)$ and the point $x_m{}^k$ has the lowest probability value of $2/(m(m+1))$

**3)** Randomly choose $q$ distinct points $u_1,\ldots,u_q$ from a complex $A^k$ to form a subcomplex using the probability distribution specified in (2). Store them in array $B = \{u_i, v_i, i = 1,\ldots,q\}$ , where $v_j$ is the function value associated with point $u_i$. Store the locations of $A^k$ which are used to construct $B$ in $L$.

**4)** Generate offsprings according to the following procedure:

**a.** Sort $B$ and $L$ so that the $q$ points are arranged in order of increasing function value and compute the centroid $g$ of the best $q$-1 points using the expression:

$$g = \frac{1}{q-1}\sum_{j=1}^{q-1} u_j \tag{5.3}$$

**b.** Execute a reflection step by computing a new point $r$ as $r = 2g - u_q$, where $u_q$ is the worst point in the search space.

**c.** If $r$ is within the feasible parameter space $\Omega$ compute the function value $f_r$ and go to step d; otherwise compute the smallest hypercube $H \subset \Re^n$ that contains $A^k$, randomly generate a point $z$ within $H$, compute the function value $f_z$, set $r = z$ and set $f_r = f_z$ (mutation step)

**d.** If $f_r < f_q$ replace $u_q$ by $r$, go to step $f$; otherwise perform a contraction step by computing a point $c$ as $c = 0.5(q + u_q)$ and calculate $f_c$.

**e.** If $f_c < f_q$, replace $u_q$ by $c$, go to step f; otherwise randomly generate a point $z$ within $H$ and compute $f_z$ (mutation step). Replace $u_q$ by $z$.

**f.** Repeat steps a - e $\omega$ times.

**5)** Replace parents by offsprings by putting the contents of $B$ into $A^k$ using the original locations stored in $L$. Sort $A^k$ in order of increasing function value.

**6)** Repeat steps 2-5 $\beta$ times.

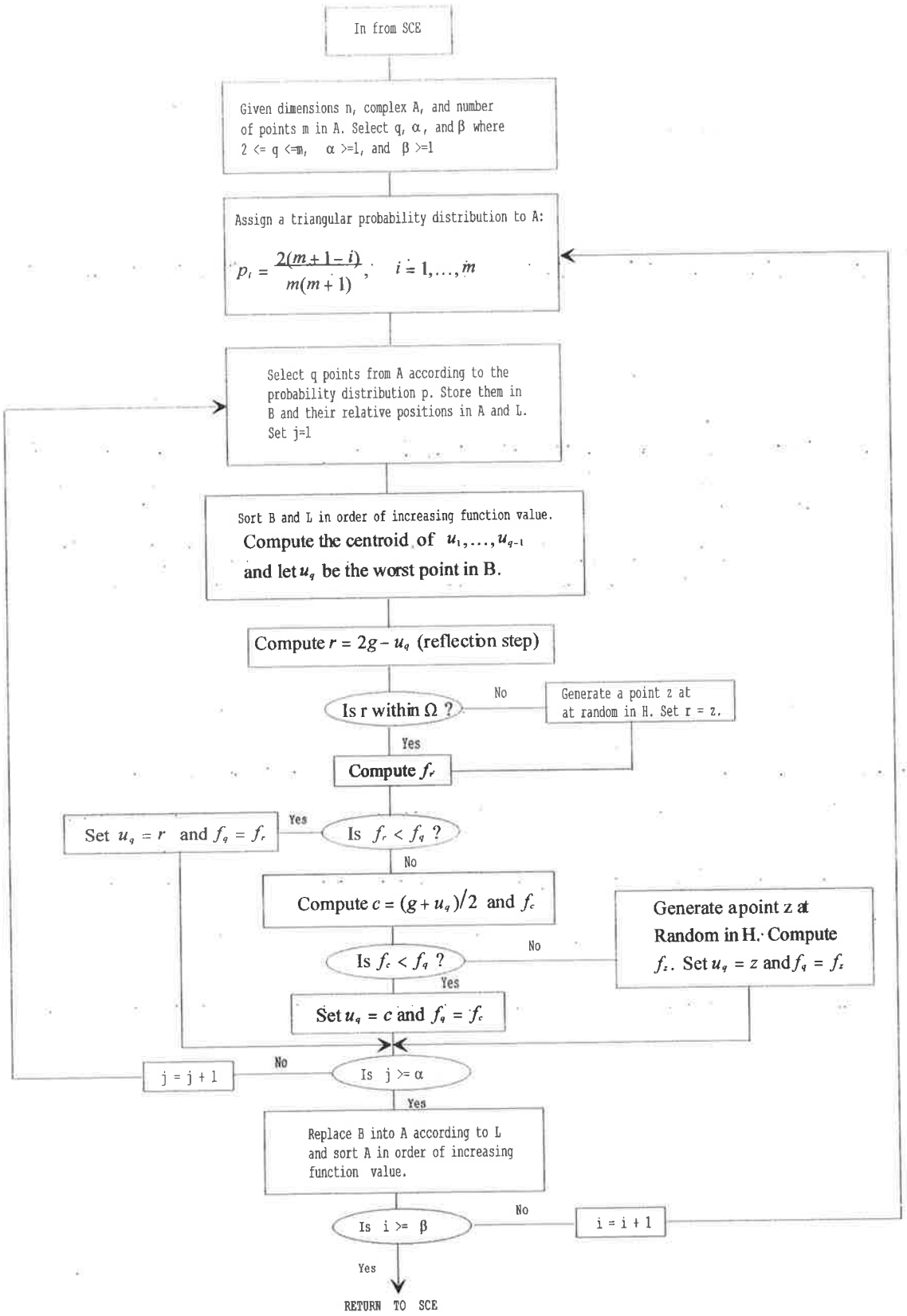



**Figure 5.9** Schematic representation of the CCE algorithm

The SCE method considers the global search as a natural evolution process where a population is partitioned into several communities (or complexes); each of which is permitted to generate offsprings independently. New communities are formed through a process of shuffling after a certain number of offspring generations. The shuffling process permits the sharing of information gained independently by each community during the evolutionary process. A competitive evolution process is guaranteed through a recognition of the fact that parents with higher probabilities contribute more to the generation of offsprings than those with lower probabilities. Such competitiveness is ensured by the use of triangular probability distribution. Generation of an offspring from a subcomplex is analogous to the crossover operation of genetic algorithms. However, the major difference between the two is that while all parents of a subcomplex are allowed at least once to take part in the generation of offsprings in the context of the SCE methodology, some parents with low fitnesses, in the context of GAs, may not be permitted to take part in the generation of offsprings. Therefore while the GA looses some information contained in the sample space, the SCE does not.

### 5.3.3 Selection of Algorithmic Parameters

The number of input parameters to the SCE algorithm is relatively few. However, the choice of these parameters is required to be made with care in order to obtain optimal results from the algorithm. The required parameters by the SCE methodology are : (1) $m$, the number of points in a complex, (2) $q$, the number of points in a subcomplex, (3) $p$, the number of complexes, (4) $p_{\min}$, the minimum number of complexes required in a population, (5) $\omega$, the number of consecutive offspring generated by each subcomplex, and (6) $\beta$, the number of evolution steps taken by each complex. In fact for some problems the proper selection of these parameters can be difficult. In view of this, *Duan et al.* [1994]

presented a comprehensive report on the proper selection of the SCE optimisation parameters and recommended the following:

$$\begin{aligned} m &= 2n+1 \\ q &= n+1, \\ \beta &= m, \\ \omega &= 1, \\ p &= p_{\min} \end{aligned} \tag{5.4}$$

where $n$ is the number of parameters being estimated (or problem dimension). The use of these recommended values reduces the burden of parameter selection to only $p$ - the number of complexes - as input to the SCE model in the present research work. *Duan et al.* [1994] pointed out the right value of $p$ depends on the degree of difficulty and the dimensionality of the problem under consideration.

### 5.3.4 Objective Function (or Calibration Criterion)

A number of different techniques have been proposed for the estimation of the parameters of a model given limited observed data. All these techniques have one goal in common. The goal of any calibration model is to identify those values of the model parameters that minimise (or maximise, if appropriate) some specified function relating the measured data and the corresponding simulated results by the model. A measure of the fit between the simulated and the observed data through the adjustment of the parameters of the simulation model is called the objective function or the calibration criterion.

Traditionally, adjustment of the model parameters have been pursued through a trial-and-error technique that requires the experience and expertise of the hydrologist or the practicing engineer on the model under consideration. In the SCE methodology the

adjustment of parameters is done automatically through the competitive complex evolution algorithm through replacement of the weaker members of the subcomplex with healthier generated offspring. Once the objective function attains its optimum value, the corresponding parameters are considered as the optimum estimated parameter values with respect to the observed data provided.

The objective function to be minimised in this work is the sum of the least squared error between the observed and the corresponding simulated data. This may be expressed mathematically as:

$$f(x_1,..,x_n) = \text{minimize}\left(\sum_{k=1}^{nobs}(h_k{}^{obs} - h_k{}^{sim})^2\right) \tag{5.5}$$

subject to $x_{li} \le x_i \le x_{ui}, \quad i = 1,2,...,n$

where

| | |
|---|---|
| $f$ | objective function, |
| $x_i$ | model parameter $i$, |
| $nobs$ | number of data points (observed or measured data), |
| $h_k{}^{obs}$ | measured or observed data value at node $k$, |
| $h_k{}^{sim}$ | corresponding simulated data value at node $k$, |
| $x_{li}$ | lower limit of parameter $x_i$, |
| $x_{ui}$ | upper limit of parameter $x_i$, and |
| $n$ | total number of variables being estimated. |

Two- and three-dimensional finite element models have been designed for the simulation of the values of $h_k{}^{sim}$. The governing equations of the two- and three-dimensional finite element models, including their formulation, and solution techniques have been presented in

chapter four. The objective function presented in equation (5.4) is in fact general and any of the flow or solute transport models presented in chapter four (be it two- or three-dimensional) can be used for the evaluation of $h_k^{sim}$ in the inverse problem of parameter identification.

## 5.4 Summary

This chapter has presented two evolutionary techniques: (1) genetic algorithm and (2) shuffled complex evolution, and their subsequent formulations for the two projects proposed in this research work. The genetic algorithm is designed to be linked with a two-dimensional finite element model of flow and solute transport in nonhomogeneous confined or unconfined aquifers for the optimisation of extraction of contaminants in polluted aquifers. The shuffled complex evolution is designed as a stand-alone inverse model that can link up with analytical models, and two- or three-dimensional flow and solute transport finite element for aquifer parameter estimation. These techniques are tested with analytical models (before their implementation with numerical models) in chapter six.

# Chapter 6

# Evaluation and Verification of Models

## 6.1 Introduction

Good programming practice requires a thorough testing or evaluation of developed models before their application to field-scale problems. Therefore this chapter deals with the evaluation of the developed models using some simple pumping test and synthetic data. The models designed may be categorised into: (1) a parameter estimation program based on the theory of the shuffled complex evolution (SCE), and (2) a remediation design program based on the theory of genetic algorithm. In each of these models, is embedded the numerical flow and/or solute transport model. However, for the purposes of evaluation of the strengths of the optimisation routines, analytical models of flow and solute transport have been substituted for the numerical models. The analytical models are utilised for this initial testing as the run times are many orders of magnitude less than for numerical models. The specific tasks accomplished in this chapter include: (1) evaluation of the SCE inverse model using analytical solute transport models with synthesised data, (2) evaluation of the SCE inverse model using Theis analytical flow model and field pumping test data, and (3) evaluation of the two- and three-dimensional solute transport models using appropriate analytical solute transport models.

## 6.2 The Analytical Models

This section briefly introduces the definitions of the analytical models used in place of the numerical models for the SCE evaluation exercise. Three analytical models in the context of solute transport and one in the context of flow are used in this exercise. The three scenarios simulated in the context of the solute transport are shown Figure 6.1. These three models are governed by the following two-dimensional equation:

$$\frac{\partial c}{\partial t} + \frac{u}{R}\frac{\partial c}{\partial x} = \frac{D_L}{R}\frac{\partial^2 c}{\partial x^2} + \frac{D_T}{R}\frac{\partial^2 c}{\partial y^2} - \lambda c \qquad (6.1)$$

with $D_L = \alpha_L u, \quad D_T = \alpha_T u, \quad u > 0$

where

$\alpha_L$ longitudinal dispersivity [$L$],

$\alpha_T$ transverse dispersivity [$L$]

$D_L$ longitudinal dispersion coefficient [$L^2T^{-1}$]

$D_T$ transverse dispersion coefficient [$L^2T^{-1}$],

$R$ retardation factor [$L^0$],

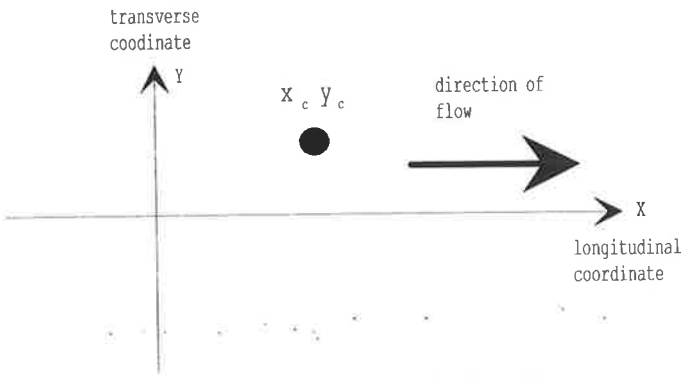
$\lambda$ degradation rate of pollutant [$T^{-1}$],

$x,y$ horizontal coordinates [$L$],

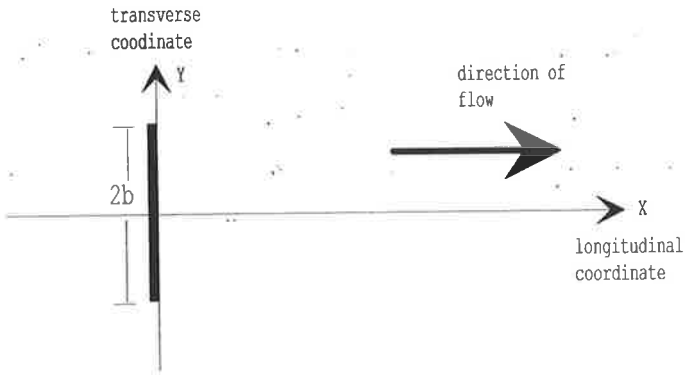
$t$ time [$T$],

$u$ unidirectional velocity in the x-direction [$LT^{-1}$], and

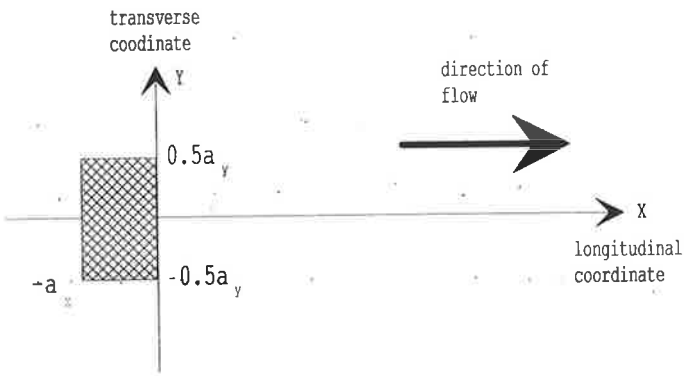
$c(x,y,t)$ concentration of pollutant [$ML^{-3}$].




a) Model 1 : Continuous point source




b) Model 2 : Exponetial decay line source




c) Model 3 : Distributed pollutant source in two-dimension

**Figure 6.1** Models used in the evaluation of the SCE algorithm

The aquifer is assumed to extend to infinity in both positive and negative x- and y-directions and the x-axis is aligned with the direction of constant velocity. The analytical solution to

equation (6.1) is obtained for each of the three different solute transport situations shown in Figure 6.1 based on their boundary and initial conditions and the type of source input.

### 6.2.1 Analytical Solution to Model 1

*Model type* : A continuous point-source of constant rate $M_o$.

*Initial and boundary conditions* :

$$c_\delta(x,y,t=0) = \frac{M_0}{\phi m R}\delta(x)\delta(y) \qquad (6.2)$$
$$c_\delta(\pm\infty,\pm\infty,t) = 0$$

where $M_0$ is the constant injection rate, $\phi$ is the effective aquifer porosity, $m$ is the aquifer thickness, and the Dirac-functions $\delta(x)$ and $\delta(y)$ are defined as:

$$\delta(x) = \delta(y) = 0 \quad \text{for } x \neq 0, \qquad \int_{-\infty}^{\infty}\delta(x) = \int_{-\infty}^{\infty}\delta(y) = 1 \qquad (6.3)$$

*Closed-form analytical solution* [*Kinzelbach*, 1986]:

$$c(x,y,t) = \frac{M_0}{4\pi\phi u\sqrt{\alpha_L\alpha_T}}\int_0^{\frac{4\alpha_L ut}{Rr^2}}\frac{1}{\varsigma}\exp\left(\frac{1}{\varsigma}-\frac{\varsigma}{4}\left\{\frac{r}{2\alpha_L}\right\}^2\left\{1+\frac{4\lambda\alpha_L R}{u}\right\}\right)d\varsigma \qquad (6.4)$$

with $r = \sqrt{x^2 + y^2\left(\frac{\alpha_L}{\alpha_T}\right)}$

where $\varsigma$ is an integration parameter.

*Parameters estimated*: $\phi$, $\alpha_L$, and $\alpha_T$.

## 6.2.2 Analytical Solution to Model 2

*Model type :* Time-varying specified line concentration source

*Boundary condition*:

$$\begin{aligned} c(0,y,t) &= c_0 e^{-\kappa t} \quad \text{for} \quad -b \le y \le b \\ c(0,y,t) &= 0 \quad \text{elsewhere} \end{aligned} \tag{6.5}$$

where $\kappa$ is the specified concentration decay factor. For $\kappa$=0, the first equation in (6.5) reduces to a specified constant concentration ( or Dirichlet's boundary condition) of value $c_0$. The length of the line source is *2b*.

*Closed-form analytical solution* [*Cleary and Ungs*, 1978]:

$$\begin{aligned} c(x,y,t) = \frac{c_0 x}{4\sqrt{\pi D_L}} \exp\left(\frac{ux}{2D_L} - \kappa t\right) \int_0^{\frac{t}{R}} \exp\left(-\left\{\lambda R - \kappa R + \frac{u^2}{4D_L}\right\}\tau - \frac{x^2}{4D_L\tau}\right) \tau^{-\frac{3}{2}} \\ * \left(erf\left\{\frac{b-y}{2\sqrt{D_T\tau}}\right\} + erf\left\{\frac{b+y}{2\sqrt{D_T\tau}}\right\}\right) d\tau \end{aligned} \tag{6.6}$$

where $c_0$ is a constant concentration value , $\tau$ is an integration parameter and *erf* is the error function.

*Parameters estimated* : $\kappa$, $\alpha_L$, and $\alpha_T$.

### 6.2.3 Analytical Solution to Model 3

*Model Type* : 2-dimensional continuous injection source with a constant rate of $M_o$.

*Initial and boundary conditions*: same as in model 1

*Closed-form analytical solution* [*Kinzelbach*, 1986]:

$$c(x,y,t) = \frac{M_0}{4\phi mRa_x a_y}\int_0^t \left( erf\left\{\frac{x-u(t-\tau)/R}{2\sqrt{\alpha_L u(t-\tau)/R}}\right\} - erf\left\{\frac{x-a_x-u(t-\tau)/R}{2\sqrt{\alpha_{LT} u(t-\tau)/R}}\right\}\right) \left( erf\left\{\frac{y+0.5a_y}{2\sqrt{\alpha_T u(t-\tau)/R}}\right\} - erf\left\{\frac{y+0.5a_y}{2\sqrt{\alpha_T u(t-\tau)/R}}\right\}\right) \exp(-\lambda(t-\tau))d\tau \quad (7)$$

where $a_x$ and $a_y$ are the horizontal and lateral extents, respectively of the rectangular input source.

*Parameters estimated* : $\phi$, $\alpha_L$, and $\alpha_T$

It is important to emphasise that each of the analytical models defined above are used in the evaluation of the least squared objective function defined in chapter five and which will be recalled once again as

$$f(u_1,..,u_n) = \text{minimize}\left(\sum_{k=1}^{nobs}(c_k{}^{obs} - c_k{}^{sim})^2\right) \quad (6.8)$$

subject to $u_{li} \le u_i \le u_{ui}, \quad i = 1,2,\ldots,n$

where :

$f$ objective function,

$u_i$ model parameter $i$ ,

$nobs$ number of data points (observed or measured data),

$c_k^{obs}$ measured or observed concentration value at node $k$ [ $ML^{-3}$ ],

$c_k^{sim}$ corresponding simulated concentration value at node $k$ [ $ML^{-3}$ ],

$u_{li}$ lower limit of parameter $u_i$ ,

$u_{ui}$ upper limit of parameter $u_i$ , and

$n$ total number of variables being estimated.

Simulated $c_k^{sim}$ values are evaluated by the analytical solute transport models discussed above.

## 6.3 Presentation of Tests and Results

The first three tests with the solute transport models are executed using synthesised concentration data for the three solute transport scenarios shown in Figure 6.1. Synthetic concentration data is considered to be noise-free and therefore appropriate for testing the strength of an optimisation algorithm . The objective of all the three tests is to estimate the 'global optimum' using the synthesised data as observed system states. In other words if $\phi = 0.25$, $\alpha_L = 25.0$, and $\alpha_T = 5.0$ are used to generate the observed data, then these parameters values are the 'global optimum' that must be sought for with the generated observed data (or system states). Only the upper and lower limits of the parameters under estimation are required as input to the model, and the final estimated parameters will always

lie within the upper and lower limits provided. Each of the test on the three solute transport models are considered in the following section.

### 6.3.1 Test of the SCE technique with Model 1

A noise-free concentration data is synthesised for the model shown in Figure 6.1a using the following parameter values : $\alpha_L = 20.0$, $\alpha_T = 5.0$, and $\phi = 0.15$. Synthesised data is evaluated at the point [1.0m,1.0m] of the simulation region for t =100, 200,...,3000 days. The use of a noise-free data implies that the global optimum of the objective function (or the criterion value) in equation (6.8) must be zero; when this happens the optimum estimated parameters must be the same as those used to synthesise the observed data. This zero value is hardly achieved owing to the precision (machine dependent) of the values of the parameters estimated. Therefore an alternative convergence criterion for ending the simulation requires the simulation to stop if the value of the objective function does not change within a given percentage $\gamma$, for a certain number $nf$, of successive function evaluations. $\gamma$ and $nf$ are user specified values. The other fixed input parameters required by the analytical models (and not estimated with the SCE) are shown in Table 6.1.

The SCE input parameters which include the number of complexes $p$; the number of points in a complex $m$; the number of points in a subcomplex $q$; the minimum number of complexes required in a population, $p_{\min}$; the number of consecutive offspring generated by each subcomplex $\omega$; and the number of evolution steps taken by each complex, $\beta$ are fed in as input using the expression in equation (5.4) as follows:

$m = 7$, $q = 4$, $\omega = 1$, $\beta = 7$, $\omega = 1$ and $p_{\min} = p$

From equation (5.4) it can be observed that when the number of parameters under estimation $n$ is known, the SCE parameters $m$, $q$, and $\beta$ can be evaluated. However, the

number of complexes must be carefully selected in order to initialise the appropriate number of the population of points in the parameter search space. For simple analytical models (and homogeneous situation for numerical models) where the number of parameters under estimation are relatively few, $p = 2$ , have always been found to be adequate to solve the problem. Thus in this and the subsequent analyses to follow the same values of SCE input parameters defined above are used.

Four runs, each with a different but reasonable parameter limits are performed to demonstrate the search power of the SCE technique for different starting parameter ranges. The parameter limits are shown in Table 6.2. The results obtained for the four runs are summarised in Table 6.3., which contains the final estimated parameters and the mean concentration error (mcerr) for each run. The 'mcerr' is the measure of the average absolute deviation between the observed and the corresponding predicted concentrations values (using the final estimated parameters).

Considering the parameter ranges used in Table 6.2 one can conclude from the results in Table 6.3 that the SCE search technique is efficient and robust. The ranges of parameter values used to estimate the parameters in Model 1 indicates that the technique has the capability to search for the optimum solution irrespective of parameter limits set for the problem. It is appropriate to mention that for all the ranges of parameters used in Table 6.2, only two complexes were required to yield the desired results for each of the runs. This is due to the fact that the number of parameters under estimation is only three. For a higher dimensions problem, two complexes may not be enough to yield the desired results.

**Table 6.1** Values of other parameters used in the analyses

| Parameter | Value |
|---|---|
| Specified concentration [$mgl^{-1}$] | 1.0 |
| Decay coefficient ($\lambda$) [1/day] | 1.65e-5 |
| Retardation coefficient (R) | 1.0 |
| Lateral extent of solute source (2b or $a_y$) [$m$] | 0.5 |
| Horizontal extent of solute source ($a_x$) [$m$] | 0.5 |
| Aquifer thickness [$m$] | 1.0 |
| Unidirectional velocity (u) [$m / day$] | 1.0 |

**Table 6.2** Parameter limits used in testing Model 1

| Parameter | RUN 1 | | RUN 2 | | RUN 3 | | RUN 4 | |
|---|---|---|---|---|---|---|---|---|
| | lower limit | upper limit | lower limit | upper limit | lower limit | upper limit | lower limit | upper limit |
| $\alpha_L$(m) | 1.00 | 100.00 | 1.00 | 200.00 | 1.00 | 350.00 | 1.00 | 500.00 |
| $\alpha_T$(m) | 1.00 | 100.00 | 1.00 | 200.00 | 1.00 | 350.00 | 1.00 | 500.00 |
| $\phi$ | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 |

**Table 6.3** Results of the Estimated Parameters for Model 1

| Parameter | Expected Values | RUN 1 mcerr = 8.96E-8 | RUN 2 mcerr = 1.13E-8 | RUN 3 mcerr = 3.04E-8 | RUN 4 mcerr = 5.06E-8 |
|---|---|---|---|---|---|
| $\alpha_L$(m) | 20.0000 | 19.9873 | 19.9821 | 20.0146 | 20.0269 |
| $\alpha_T$(m) | 5.0000 | 5.0004 | 5.0003 | 5.0006 | 5.0014 |
| $\phi$ | 0.1500 | 0.1500 | 0.1501 | 0.1499 | 0.1499 |

## 6.3.2 Test of the SCE technique with Model 2

To test the SCE method with Model 2, synthesised concentration data for the scenario shown in Figure 6.1b is created using the following parameter values: $\alpha_L = 20.0$, $\alpha_T = 5.0$, and $\kappa = 0.0015$. Synthesised data is computed at the same location of the simulation region and simulation times as in model 1. The upper and lower limits of

the parameters to be estimated are as shown in Table 6.4. The SCE parameters namely the number of complexes, the number of points in a complex, the number of points in a subcomplex, the number of consecutive offsprings generated by each subcomplex, and the number of evolution steps taken by each complex are the same as those used in Model 1.

Once again four runs are performed using different parameter ranges in each run. The results of the four runs are shown in Table 6.5. It can be seen that the parameters estimated using the different initial ranges in Table 6.4 are all very close to the expected values. The values of 'mcerr' in each of the tests also support the fact the final concentration values predicted with final estimated parameters are almost the same as the corresponding observed data.

**Table 6.4** Parameter limits used in testing Model 2

| Parameter | RUN 1 | | RUN 2 | | RUN 3 | | RUN 4 | |
|---|---|---|---|---|---|---|---|---|
| | lower limit | upper limit | lower limit | upper limit | lower limit | upper limit | lower limit | upper limit |
| $\alpha_L$ (m) | 1.00 | 100.00 | 1.00 | 200.00 | 1.00 | 300.00 | 1.00 | 500.00 |
| $\alpha_T$ (m) | 1.00 | 100.00 | 1.00 | 200.00 | 1.00 | 300.00 | 1.00 | 500.00 |
| $\kappa$ (1/d) | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 |

**Table 6.5** Results of the Estimated Parameters for Model 2

| Parameter | Expected Values | RUN 1 mcerr = 1.32E-9 | RUN 2 mcerr = 3.2E-10 | RUN 3 mcerr = 8.44E-9 | RUN 4 mcerr = 4.7E-10 |
|---|---|---|---|---|---|
| $\alpha_L$ (m) | 45.0000 | 45.0278 | 44.9921 | 45.0682 | 44.9887 |
| $\alpha_T$ (m) | 30.0000 | 29.9951 | 30.0031 | 29.9997 | 30.0034 |
| $\kappa$ (1/d) | 0.0015 | 0.00149 | 0.00150 | 0.00150 | 0.00150 |

### 6.3.3 Test of the SCE technique with Model 3

Synthesised concentration data for this analysis is generated for the scenario shown in Figure 6.1c using the following values : $\alpha_L = 60.0$, $\alpha_T = 25.0$, and $\phi = 0.35$; for the same location and simulation times as in the two previous models. The SCE parameters are the same as those used in the previous two analyses. The parameter boundary limits for four runs are shown in Table 6.6 and the final estimated parameters for the runs are shown in Table 6.7. Again the final estimated parameters are very close to the expected values in column 2 of Table 6.7, despite the range of parameter limits used in Table 6.6. This conclusion is also supported by the small values of 'mcerr' shown in Table 6.7. In all the three tests various initial starting ranges have been used to demonstrate the robustness of the search power of the SCE. For the third model in particular, one can observe the very wide range with regard to the initial parameter values; yet the SCE technique was able to locate approximately the same values of the optimum parameters for all the four runs considered in this model.

**Table 6.6** Parameter limits used in testing Model 3

| Parameter | RUN 1 | | RUN 2 | | RUN 3 | | RUN 4 | |
|---|---|---|---|---|---|---|---|---|
| | lower limit | upper limit | lower limit | upper limit | lower limit | upper limit | lower limit | upper limit |
| $\alpha_L$ (m) | 1.00 | 100.00 | 1.00 | 500.00 | 1.00 | 750.00 | 1.00 | 1000.00 |
| $\alpha_T$ (m) | 1.00 | 100.00 | 1.00 | 500.00 | 1.00 | 750.00 | 1.00 | 1000.00 |
| $\phi$ | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 |

**Table 6.7** Results of the estimated parameters for Model 3

| Parameter | Expected Values | RUN 1 mcerr = 1.65E-11 | RUN 2 objv = 1.46E-8 | RUN 3 mcerr = 7.60E-9 | RUN 4 mcerr = 1.72E-8 |
|---|---|---|---|---|---|
| $\alpha_L$ (m) | 60.0000 | 59.9960 | 60.0335 | 60.0337 | 60.0202 |
| $\alpha_T$ (m) | 25.0000 | 24.9999 | 24.9874 | 24.9905 | 24.9893 |
| $\phi$ | 0.3500 | 0.3500 | 0.3500 | 0.3500 | 0.3500 |

### 6.3.4 Evaluation of the SCE Using Analytical Flow Model with Field Data

In the fourth evaluation, the Theis analytical flow model is employed in conjunction with a field experimental pumping test conducted in South Australia. The analytical model allows the assumption that the specified drawdown at an infinite location from the point of pumping is zero. It also permits the assumption that the initial drawdown within the area in which the pumping test was carried out is zero. This model may be expressed in radial coordinates as [*Kinzelbach*, 1986] :

$$\frac{S}{T}\frac{\partial s}{\partial t} = \frac{1}{r}\left(r\frac{\partial s}{\partial r}\right) \tag{6.9}$$

*Initial and boundary conditions :*

$$\begin{aligned} &s(t=0,r)=0 \\ &s(t,r=\infty)=0 \\ &\left(2\pi Tr\frac{\partial s}{\partial r}\right)\Big|_{r=0} = Q \quad \text{for} \quad t>0 \end{aligned} \tag{6.10}$$

where

| | |
|---|---|
| $r$ | radial coordinates [$L$], |
| $S$ | storage coefficient, |
| $T$ | transmissivity [$L^2T^{-1}$], |
| $t$ | time [$T$], |
| $s$ | drawdown [$L$], and |
| $Q$ | withdrawal rate starting at time $t = 0$ |

Combining equations (6.9) and (6.10), the Theis analytical solution is expressed as [*Kinzelbach*, 1986]:

$$s(t,r)=\frac{Q}{4\pi T}W(u),\quad u=\frac{Sr^2}{4Tt},\quad W(u)=-0.5771-\ln(u)+u-\frac{u^2}{2x\,2!}+\ldots. \qquad (6.11)$$

*Parameters estimated* : *SC* and *TS*

The SCE model was tested on a field pumping test experiment conducted in South Australia, together with two other models, GALG and GNEW. GALG is a parameter estimation model whose principle is based on the theory of genetic algorithms presented in chapter five while GNEW is based on the Gauss-Newton gradient-based technique. These two models have been designed in the course of this research study for the evaluation of the experimental pumping test data with respect to parameter estimation. Hence, the secondary objective in this section in particular, is to investigate how the results of the evolutionary models compare with those of a traditional gradient-based method. Three series of data are used. For convenience they are referred to as TEST1, TEST2, and TEST3. Data TEST1 were collected with the production well operating at the rate of 21 $ls^{-1}$ and the observation well located at a radial distance of 25 *m* from the production well; data TEST2 were collected with the production well operating at the rate of 9 $ls^{-1}$ with the observation again at a radial distance of 25 *m* from the production well; and data TEST3 had the observation well located at 65 *m* from the production well, with the latter operating at the rate of 9 $ls^{-1}$.

All the three experiments were conducted on different occasions but using the same pumping well with the observation or test wells in the same straight line. Using these three data sets and assuming a homogenous isotropic aquifer, three inverse analyses were performed for each of the three data sets using the Theis analytical flow model discussed previously. The parameters estimated are the effective storage coefficient (*SC*) and the effective transmissivity (*TS*).

The lower and upper limits of these parameters used in each of the three models for the three data sets are shown in Table 6.8. It is apparent in this table that the limits used is model-dependent. Each model has its unique range for which meaningful results could be obtained. While the GNEW model could search within a wider range (at the expense of excessive computational time), the GALG model required a smaller range to perform its search. The final range for the GA was determined after initial analyses with larger ranges which did not produce adequate convergence. The range of the SCE model depends on the number of complexes. In this particular problem the use of 2 complexes required the appropriate range shown in Table 6.8 for a more meaningful results. It is appropriate to mention that the SCE has the capacity to accommodate a wider range if required (this has been illustrated in the previous examples with the solute transport models).

**Table 6.8** Parameter limits used in all the three tests

| | SCEV | | GNEW | | GALG | |
|---|---|---|---|---|---|---|
| Parameter | lower | upper | lower | upper | lower | upper |
| *SC* | 1.0e-10 | 1.0 | 1.0e-10 | 1.0 | 0.1e-3 | 0.1e-4 |
| *TS* $[m^2 s^{-1}]$ | 1.0e-10 | 1.0 | 1.0e-10 | 100.0 | 0.5e-2 | 0.5e-4 |

**Table 6.9** Final Estimated Parameters

| | TEST1 | | TEST2 | | TEST3 | |
|---|---|---|---|---|---|---|
| Model | *SC* | *TS* $[m^2 s^{-1}]$ | *SC* | *TS* $[m^2 s^{-1}]$ | *SC* | *TS* $[m^2 s^{-1}]$ |
| SCEV | 0.2377e-4 | 0.20639e-2 | 0.1475e-4 | 0.21530e-2 | 0.3889e-3 | 0.19045e-2 |
| GNEW | 0.2373e-4 | 0.20639e-2 | 0.1487e-4 | 0.21500e-2 | 0.3893e-3 | 0.19041e-2 |
| GALG | 0.1871e-4 | 0.21258e-2 | 0.1342e-4 | 0.21265e-2 | 0.3668e-3 | 0.20180e-2 |

**Table 6.10** Comparison of models performance using coefficient of correlation

| Model | TEST1 | TEST2 | TEST3 |
|---|---|---|---|
| SCEV | 0.996502 | 0.982865 | 0.999131 |
| GNEW | 0.996528 | 0.982721 | 0.999130 |
| GALG | 0.996486 | 0.982679 | 0.999101 |

The final estimated parameters obtained from each of the three models based on the three pumping tests data are summarised in Table 6.9. The results reveal that the final optimum parameters obtained from SCE and GNEW are fairly close to each other. The

results of the GALG model deviated from the other two but compared favourably well with the observed data. This indicates that the estimated effective parameters may be truly representative of the aquifer formation with respect to the space and the time at which the pumping test experiment was carried out. The efficiency of the models are compared through the evaluation of the coefficient of correlation between the observed and predicted drawdowns (using the final estimated parameters shown in Table 6.9) for each of the three tests. As shown in Table 6.10, the SCE and the GNEW models have almost the same level of efficiency with respect to the three sets of data used.

Generally, the results obtained indicate that the evolutionary techniques can in fact perform as equally well as the deterministic gradient-based techniques. The added strength of the evolutionary techniques is the fact that they perform their search without the computation of derivatives of the dependent variable with respect to the parameters under estimation; making them more robust and efficient under conditions of high nonlinearity, and parameter sensitivity and interaction. The visual comparison of the three tests performed using each of the three models against the observed data is shown in Figures 6.2 to 6.4. It is clear from these three figures that results from all the three models are in good agreement with the observed data. However, SCE and GNEW models predicted better and closer to each other than the GALG model.

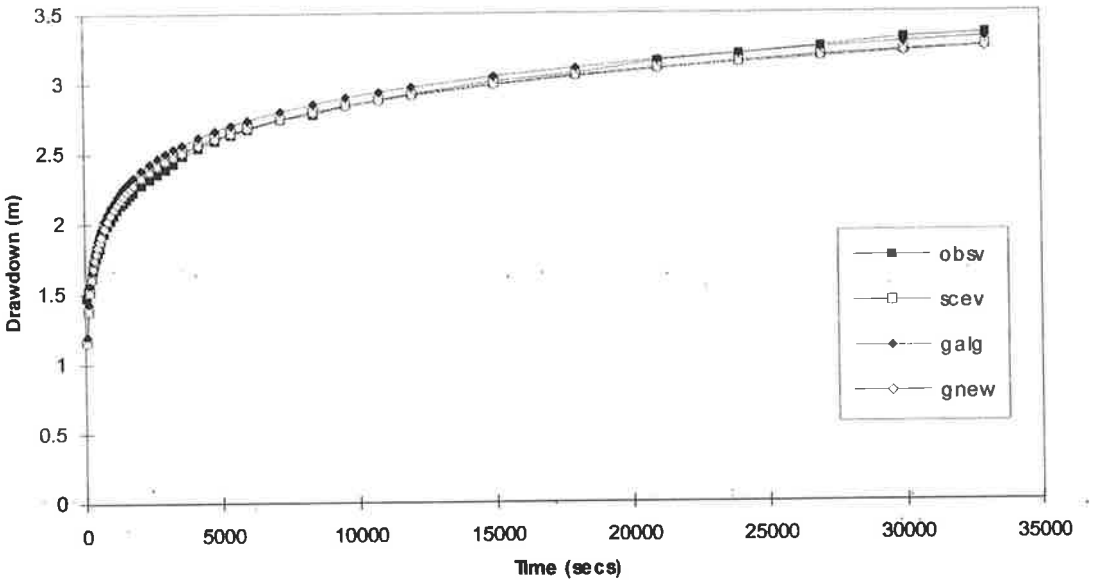



**Figure 6.2** Comparison of the efficiencies of the three techniques using data TEST1

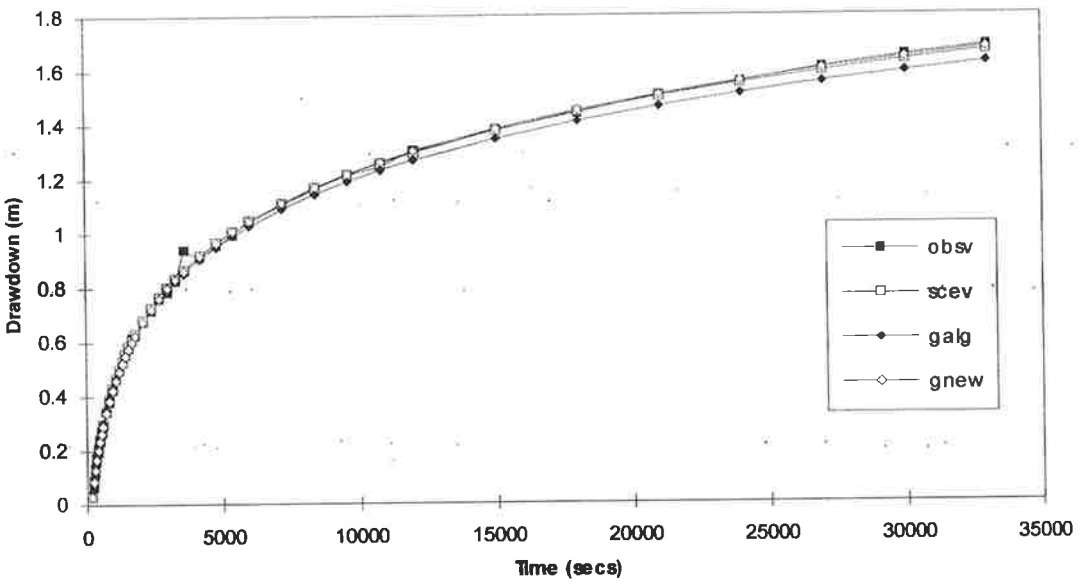



**Figure 6.3** Comparison of the efficiencies of the three techniques using data TEST2

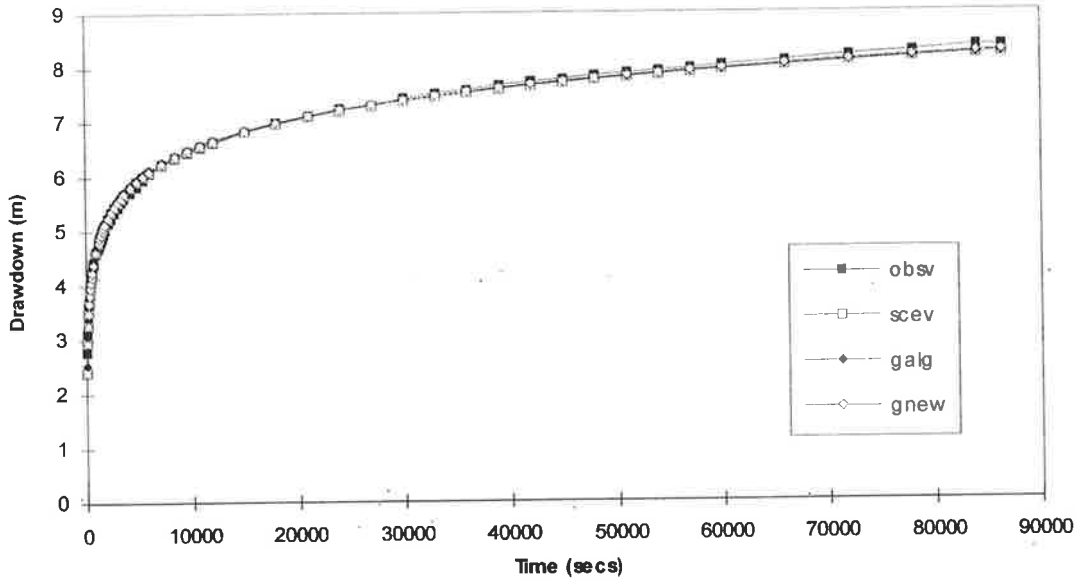



**Figure 6.4** Comparison of the efficiencies of the three techniques using data TEST3

## 6.4 Evaluation of the 2-D and 3-D Transport Models

The chapter is completed with the test of the numerical accuracy of the two- and three-dimensional finite element solute transport numerical models presented and formulated in chapter four. Because of the restrictions and assumptions imposed in order to obtain closed-form analytical solution, only simplified cases of the numerical models are tested. The analytical models chosen for this exercise are : (1) a two-dimensional model for an aquifer of infinite width with finite-width solute source, and (2) a three-dimensional model for an aquifer of infinite width and height with finite-width and finite-height solute source. The governing equations and analytical solutions to these models are presented subsequently.

### 6.4.1 Two-Dimensional Analytical Model

The two-dimensional analytical model for an aquifer of infinite width with finite-width solute source is governed by the equation:

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - V\frac{\partial C}{\partial x} - \lambda C, \text{ with } D_x = \alpha_L V,\ D_y = \alpha_T V \qquad (6.12)$$

subject to the following boundary and initial conditions:

*Boundary conditions:*

$$\begin{aligned} &C = C_0, \quad x = 0 \text{ and } Y_1 < y < Y_2 \\ &C = 0, \quad x = 0 \text{ and } y < Y_1 \text{ or } y > Y_2 \\ &C,\ \frac{\partial C}{\partial y} = 0 \text{ at } y = \pm\infty, \quad C,\frac{\partial C}{\partial x} = 0 \text{ at } x = \infty \end{aligned} \qquad (6.13)$$

*Initial conditions:*

$$C(x,y,t=0) = 0 \text{ at } 0 < x < \infty \text{ and } -\infty < y < +\infty \qquad (6.14)$$

where:

| | |
|---|---|
| $C$ | solute concentration [ $ML^{-1}$ ], |
| $V$ | fluid velocity in the x-direction [ $LT^{-1}$ ], |
| $D_x$ | longitudinal dispersion coefficient [ $L^2T^{-1}$ ], |
| $D_y$ | transverse dispersion coefficient [ $L^2T^{-1}$ ], |
| $\alpha_L$ | longitudinal dispersivity [$L$], |
| $\alpha_T$ | transverse dispersivity [$L$], |
| $\lambda$ | first-order solute decay coefficient [ $T^{-1}$ ], |
| $Y_1$ | y-coordinate of lower limit of solute source at x=0 [$L$], |

$Y_2$ y-coordinate of the upper limit of solute source at x=0 [$L$], and

$x,y$ Cartesian x- and y- coordinates of the simulation region [$L$].

The analytical solution to equation (6.12) subject to the boundary and initial conditions in equations (6.13) and (6.14) is obtained through the recognition of the following assumptions: (1) fluid is of constant density and viscosity, (2) solute may be subjected to first order chemical transformation (for a conservative solute, $\lambda$=0), (3) flow is in the x-direction only and velocity is constant, and (4) the longitudinal and transverse dispersion coefficients ($D_x$ and $D_y$) are constant. The analytical solution is given by *Wexler* [1993] as:

$$C(x,y,t)=\frac{C_0 x}{4\sqrt{\pi D_x}}\exp\left(\frac{Vx}{2D_x}\right)\int_{\tau=0}^{\tau=t}\tau^{-\frac{3}{2}}\exp\left[-\left(\frac{V^2}{4D_x}+\lambda\right)\tau-\frac{x^2}{4D_x\tau}\right]* \left\{erfc\left[\frac{Y_1-y}{2\sqrt{D_y\tau}}\right]-erfc\left[\frac{Y_2-y}{2\sqrt{D_y\tau}}\right]\right\}d\tau \tag{6.15}$$

where *erfc* is the complementary error function and $\tau$ is an integration parameter. *Wexler* [1993] suggested that the accuracy of the numerical integration can be improved by making a variable transformation of the form $\tau=r^4$. This transforms equation (6.15) to a final form:

$$C(x,y,t)=\frac{C_0 x}{4\sqrt{\pi D_x}}\exp\left(\frac{Vx}{2D_x}\right)\int_{r=0}^{r=t^{0.25}}\frac{1}{r^3}\exp\left[-\left(\frac{V^2}{4D_x}+\lambda\right)r^4-\frac{x^2}{4D_x r^4}\right]* \left\{erfc\left[\frac{Y_1-y}{2r^2\sqrt{D_y}}\right]-erfc\left[\frac{Y_2-y}{2r^2\sqrt{D_y}}\right]\right\}dr \tag{6.16}$$

A computer program was written to evaluate equation (6.16) using the Gauss-Legendre method of numerical integration. A simple input data was constructed for the purposes of

comparing the results of equation (6.16) to those obtained from a two-dimensional numerical solute transport model presented in chapter four.

The region simulated is shown in Figure 6.5. The region is discretized into 31 nodes along the x-direction and 15 nodes along the y-direction using the following spatial discretization scheme: $x$ = 0.0, 100.0, 200.0,...,3000.0$m$ and $y$ = 0.0, 100.0, 200.0,..., 1500.0$m$. A constant concentration source ($C_0$) at $x$ = 0 and along the range $Y_1 < y < Y_2$ (where $Y_1 = 400m$ and $Y_2 = 1000m$) is specified at a value of $100mgl^{-1}$; leading to the set up of a symmetrical problem. The simulation is performed for the times t = 10.0, 20.0,...,300.0 days.

The contours of spatial concentration distribution for both models at time t = 1000 days are shown in Figures 6.6 and 6.7. From these figures, it can be observed that the results for these two models compare favourably well. A more detailed comparison of the results from these two models on a point-by-point basis are illustrated by the breakthrough curves shown in Figures 6.8 to 6.10 for the three observation points shown in the simulation region. Once again, it can be observed from these two figures that the comparison between the results of the two models is excellent. It is appropriate to mention that the observation nodes 2 and 3 were chosen such that the two nodes could pose as mirror images of each other. This situation is confirmed both in the analytical and numerical results shown in Figures 6.9 and 6.10 by the fact that the same magnitudes of concentration values are obtained with regard to the breakthrough curves at nodes 2 and 3.

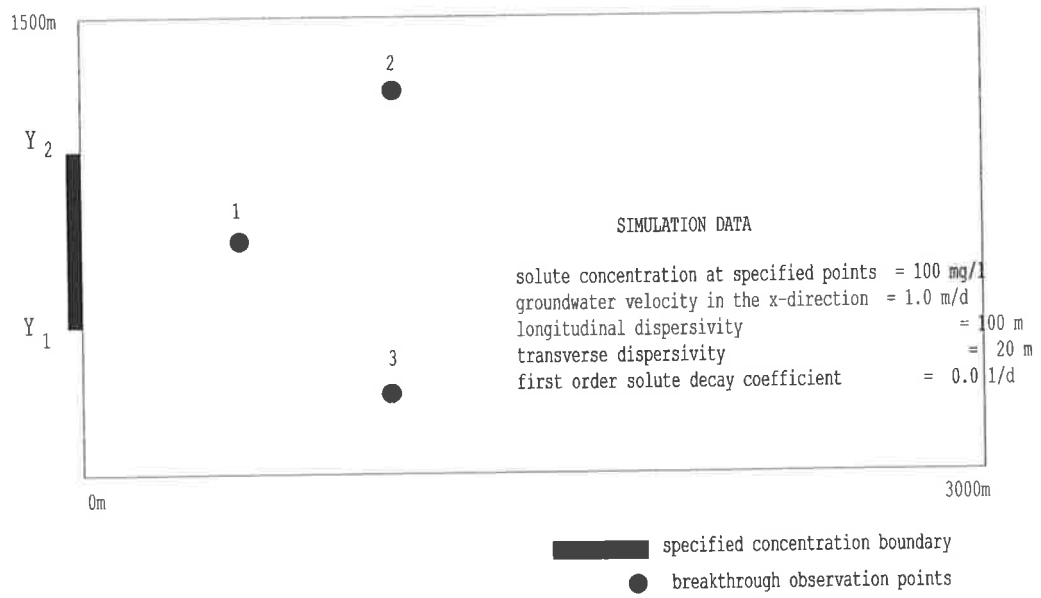



**Figure 6.5** Simulation region used for the evaluation of the 2-dimensional numerical model

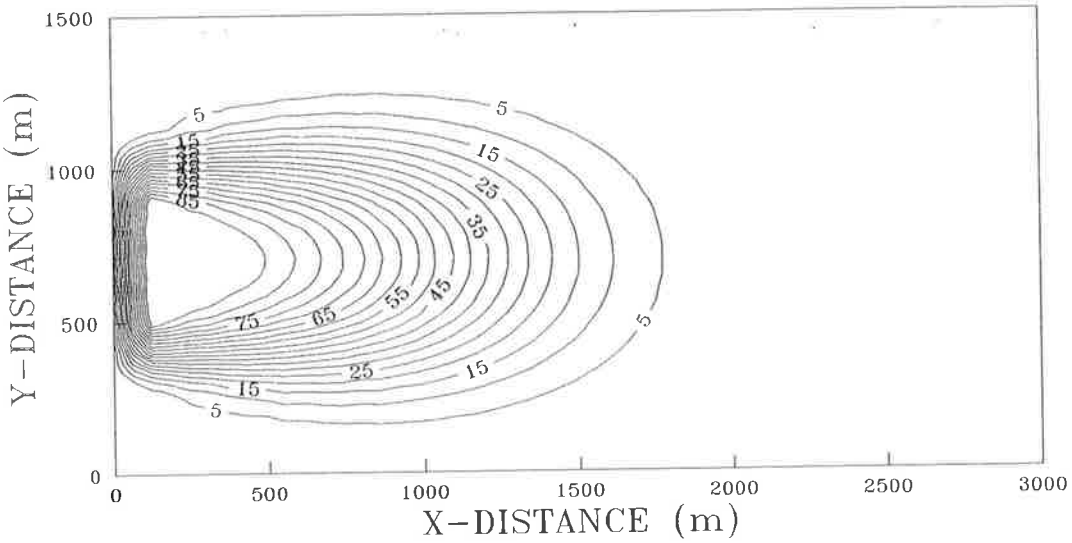



**Figure 6.6** Results of spatial concentration distribution at t=1000 days from the analytical model

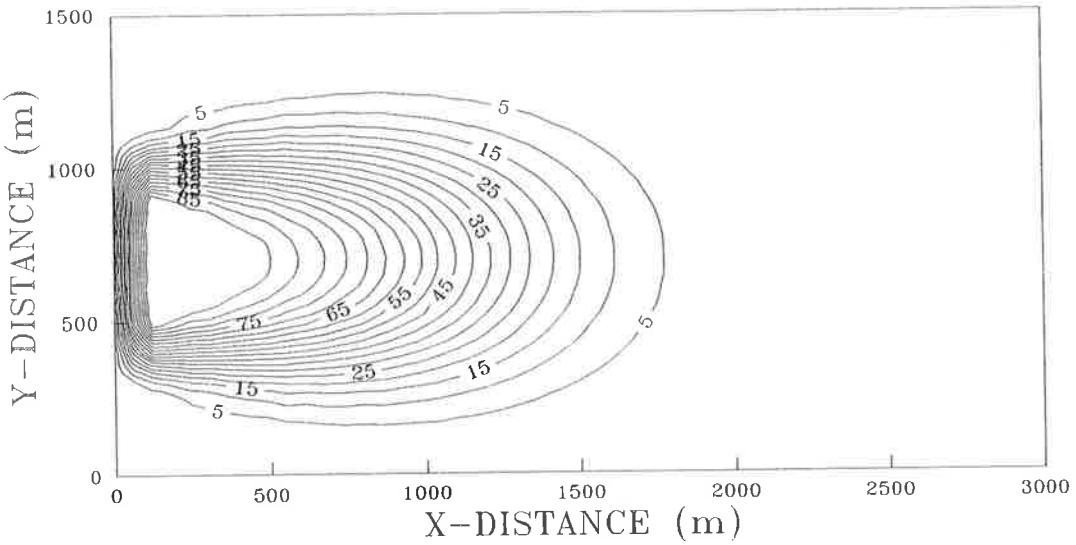



**Figure 6.7** Results of spatial concentration distribution at t=1000 days from the numerical model

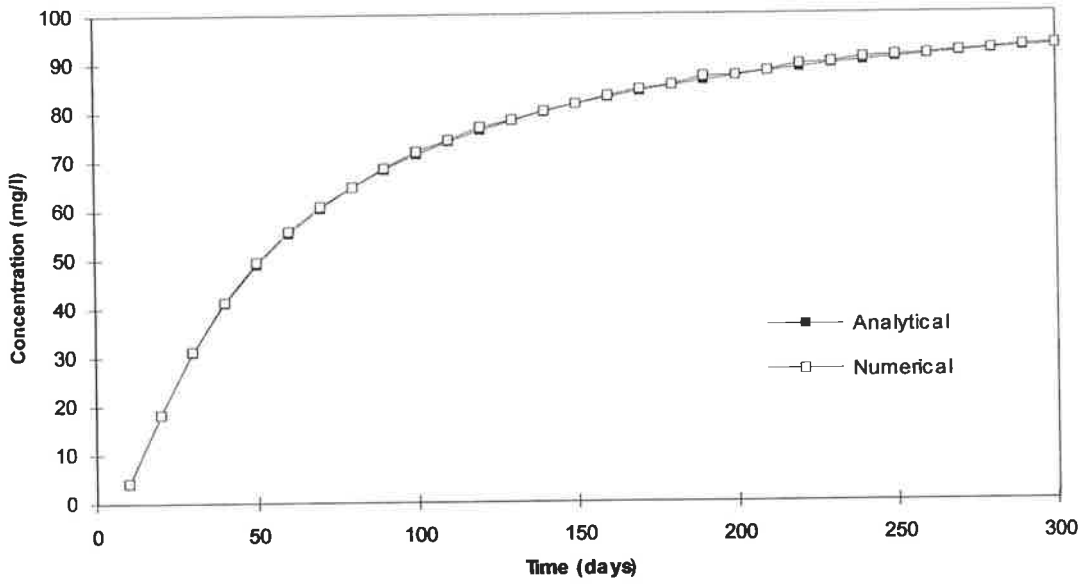



**Figure 6.8** Model evaluation using breakthrough data at observation node 1

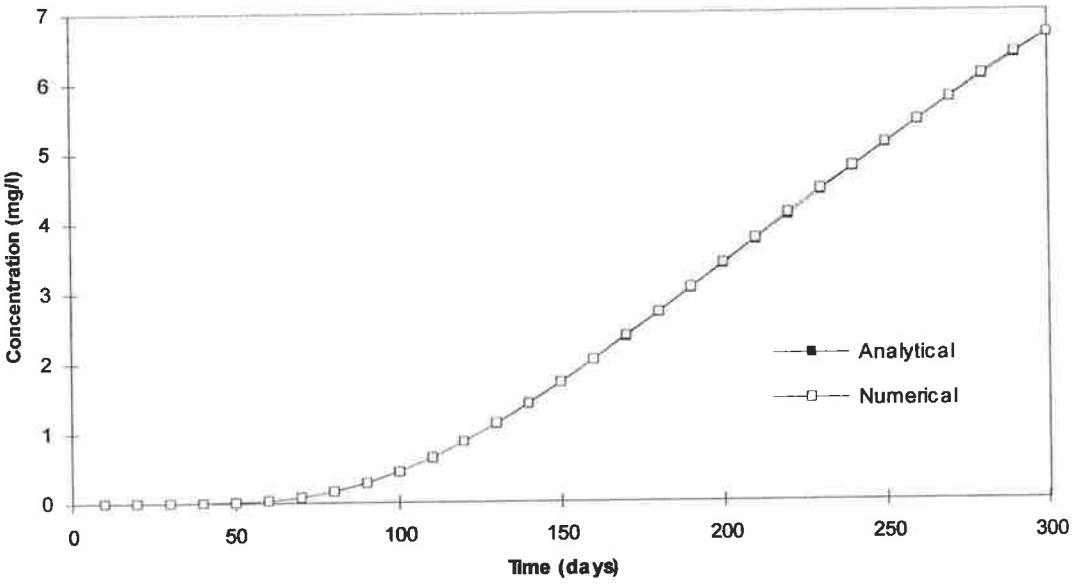



**Figure 6.9** Model evaluation using breakthrough data at observation node 2

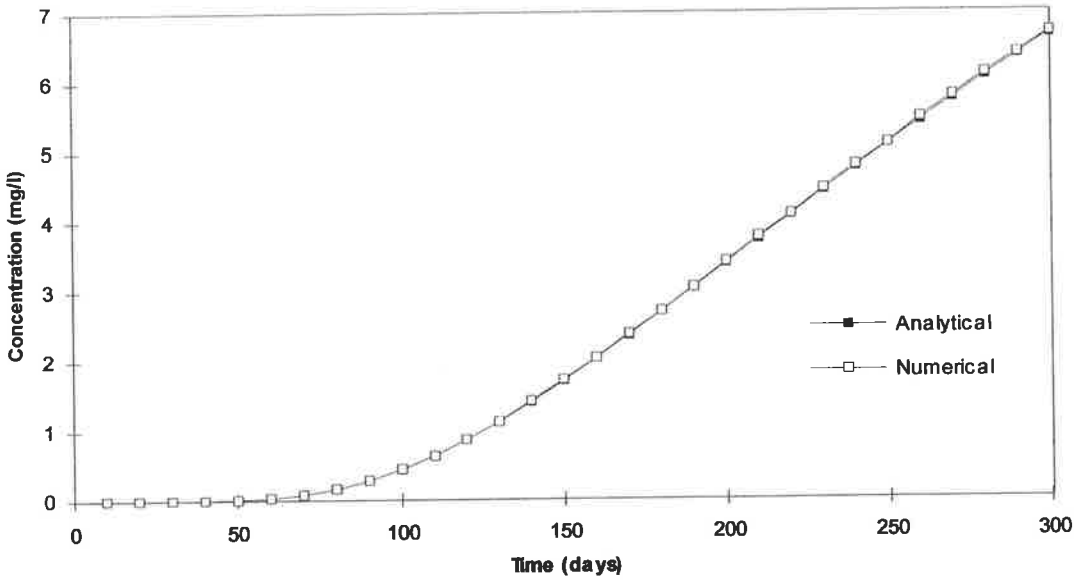



**Figure 6.10** Model evaluation using breakthrough data at observation node 3

## 6.4.2 Three-Dimensional Analytical Model

The three-dimensional analytical model governing an aquifer of infinite width and height with finite-width and finite-height solute source may be expressed as:

$$\frac{\partial C}{\partial t} + D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - V \frac{\partial C}{\partial x} - \lambda C = 0 \qquad (6.17)$$

subject to the following boundary and initial conditions:

*Boundary conditions:*

$$\begin{aligned}
&C = C_0, && x = 0 \text{ and } Y_1 < y < Y_2 \\
&&& \text{and } Z_1 < z < Z_2 \\
&C = 0, && x = 0 \text{ and } Y_1 > y \text{ or } y > Y_2 \\
&&& \text{and } Z_1 > z \text{ or } z > Z_2 \\
&C, \frac{\partial C}{\partial y} = 0, && y = \pm\infty \\
&C, \frac{\partial C}{\partial z} = 0, && z = \pm\infty \\
&C, \frac{\partial C}{\partial x} = 0, && x = \infty
\end{aligned} \qquad (6.18)$$

*Initial condition:*

$$C(x, y, z, t = 0) = 0, \quad 0 < x < \infty, \quad -\infty < y < +\infty, \quad -\infty < z < +\infty \qquad (6.19)$$

where:

$Z_1$ z-coordinate of the lower limit of the solute source at x = 0 [$L$],

$Z_2$ z-coordinate of the upper limit of the solute source at x = 0 [$L$], and

$D_z$ vertical transverse dispersion coefficient [ $L^2T^{-1}$ ].

All the other parameters in equation (6.17) have the same meanings as those defined in the two-dimensional case. The analytical solution to equation (6.17) subject to (6.18) and (6.19) also recognises the assumptions stated for the two-dimensional analytical model in the previous section. This solution may be expressed as [*Wexler*, 1993]:

$$C(x,y,z,t) = \frac{C_0 x \exp\left(\frac{Vx}{2D_x}\right)}{8\sqrt{\pi D_x}} \int_0^t \tau^{\frac{-3}{2}} \exp\left[-\left(\frac{V^2}{4D_x}+\lambda\right)\tau - \frac{x^2}{4D\tau}\right] * \left\{erfc\left[\frac{Y_1-y}{2\sqrt{D_y\tau}}\right] - erfc\left[\frac{Y_2-y}{2\sqrt{D_y\tau}}\right]\right\}\left\{erfc\left[\frac{Z_1-z}{2\sqrt{D_Z\tau}}\right] - erfc\left[\frac{Z_2-z}{2\sqrt{D_z\tau}}\right]\right\} d\tau \quad (6.20)$$

Again the transformation $\tau = r^4$ is applied to equation (6.20) for accuracy of numerical integration. This results in the final expression:

$$C(x,y,z,t) = \frac{C_0 x \exp\left(\frac{Vx}{2D_x}\right)}{2\sqrt{\pi D_x}} \int_{r=0}^{r=\tau^{0.25}} \frac{1}{r^3} \exp\left[-\left(\frac{V^2}{4D_x}+\lambda\right)r^4 - \frac{x^2}{4Dr^4}\right] * \left\{erfc\left[\frac{Y_1-y}{2r^2\sqrt{D_y}}\right] - erfc\left[\frac{Y_2-y}{2r^2\sqrt{D_y}}\right]\right\}\left\{erfc\left[\frac{Z_1-z}{2r^2\sqrt{D_Z}}\right] - erfc\left[\frac{Z_2-z}{2r^2\sqrt{D_z}}\right]\right\} dr \quad (6.21)$$

A computer program was written to evaluate equation (6.21) using the Gauss-Legendre numerical integration technique. The three-dimensional evaluation problem handled is similar to the two-dimensional case except for the inclusion of a vertical axis. The entire simulation region is shown in Figure 6.11. The region comprises a five layered system with the horizontal specified boundaries given by $Y_1 < y < Y_2$ at x=0.0 , where $Y_1 = 400m$ and $Y_2 = 1000m$. The vertical extent of the specified boundaries are given by $Z_1 < z < Z_2$, at

x=0.0, where $Z_1 = 20m$ and $Z_2 = 40m$; resulting in the set up of a three-dimensional symmetrical problem. The value of the concentration ($C_0$) at these specified locations is $100mgl^{-1}$. The observed breakthrough points are specified within the third layer at the same locations as in the two-dimensional case.

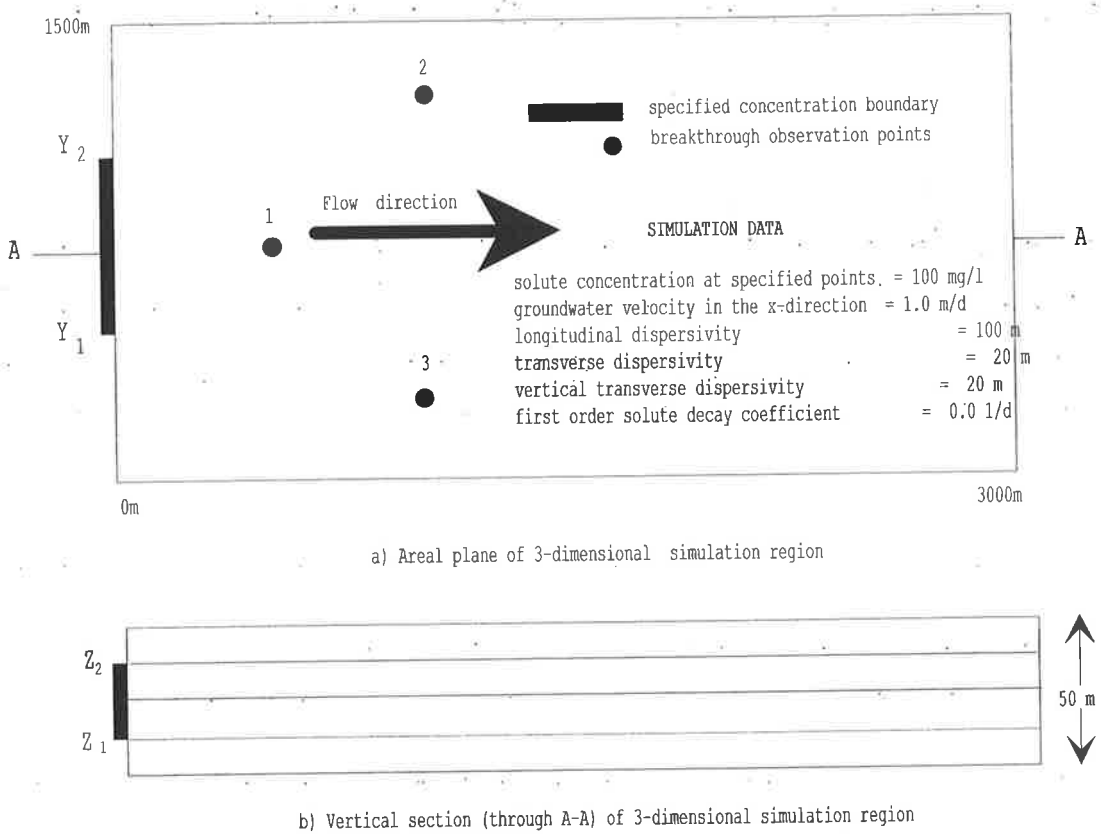



**Figure 6.11** Simulation region used for the evaluation of the 3-dimensional numerical model

The results of the concentration values at times t = 10, 20, 30,...,300 for the analytical model are compared to those of the three-dimensional model at corresponding locations. The nodal spatial discretization scheme employed is as follows: x = 0.0, 100.0, 300.0,...,3000.0m; y =0.0, 100.0, 200.0,300.0,...,1500.0m; and z = 10.0, 20.0, ..., 50.0 (the bottom of the aquifer is assumed to be at an elevation of 10.0 above some given datum).

The results of the spatial concentration distribution in the top layer of the simulation region at time t = 1500 days for both the analytical and numerical model is

shown in Figures 6.12 and 6.13, respectively. One can observed that the contours of the concentration distribution for both models compare favourably well. A critical comparison of the solutions from both model is shown by comparing the graphs of the breakthrough curves at the observation nodes in the third layer of the simulation region. A good agreement can be observed with regard to the results from the two models. The expected symmetrical results for observation nodes 2 and 3 can be observed in Figures 6.15 and 6.16.

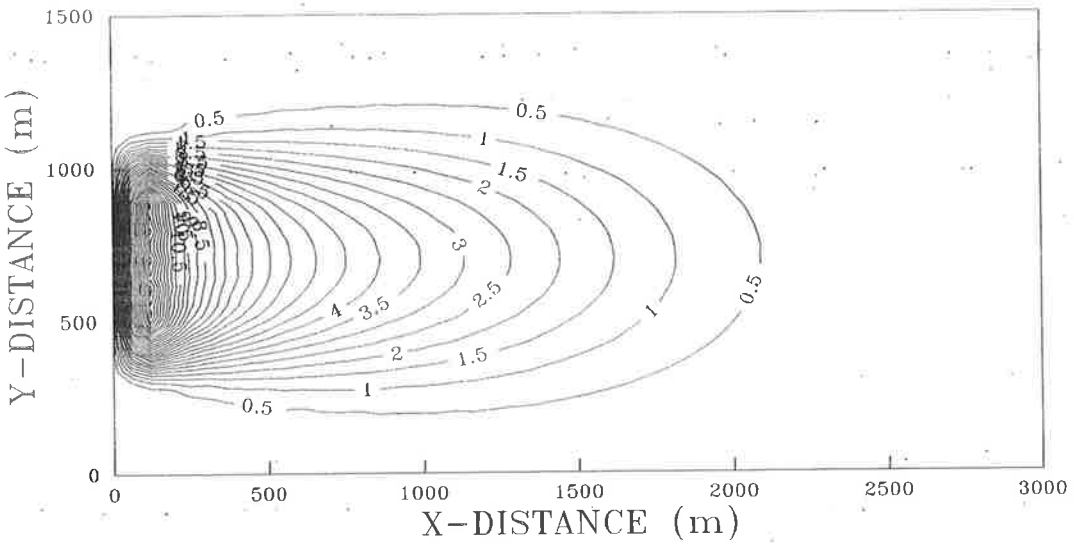



**Figure 6.12** Results of spatial concentration distribution at t=1500 days from the 3D analytical model

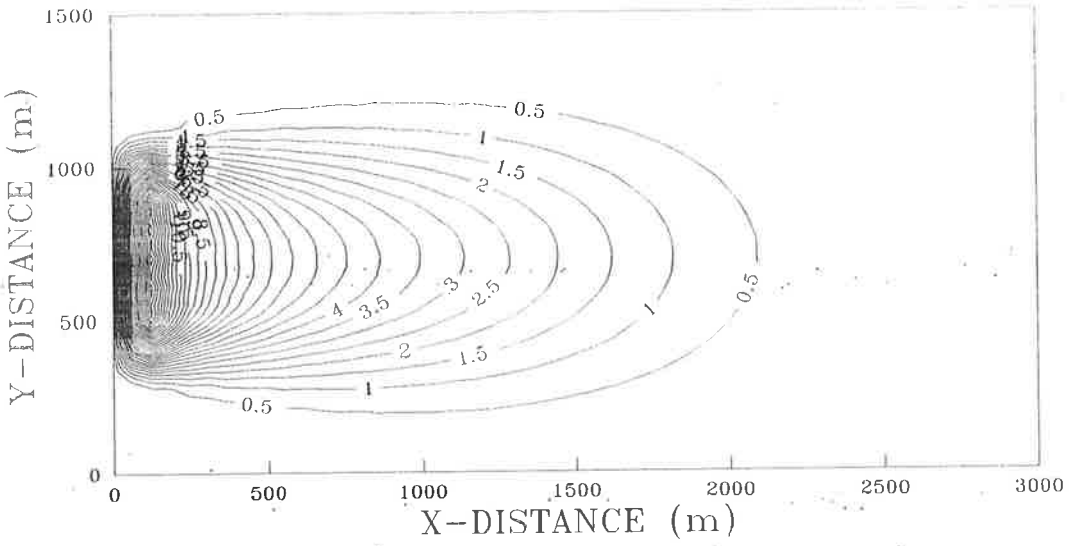



**Figure 6.13** Results of spatial concentration distribution at t=1500 days from the 3D numerical model

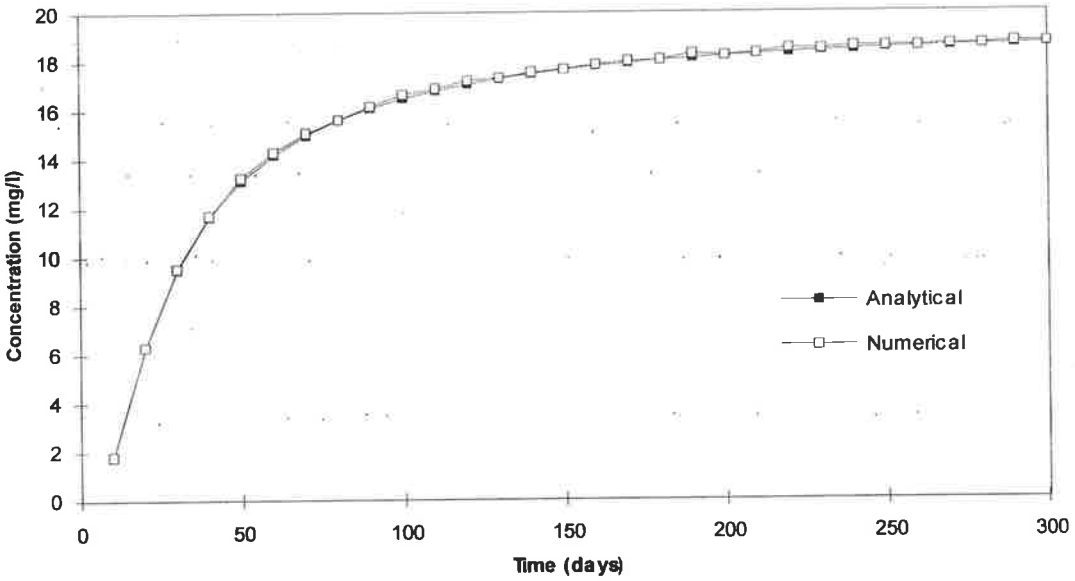



**Figure 6.14** 3-Dimensional model evaluation using breakthrough data at observation node 1 in layer 3

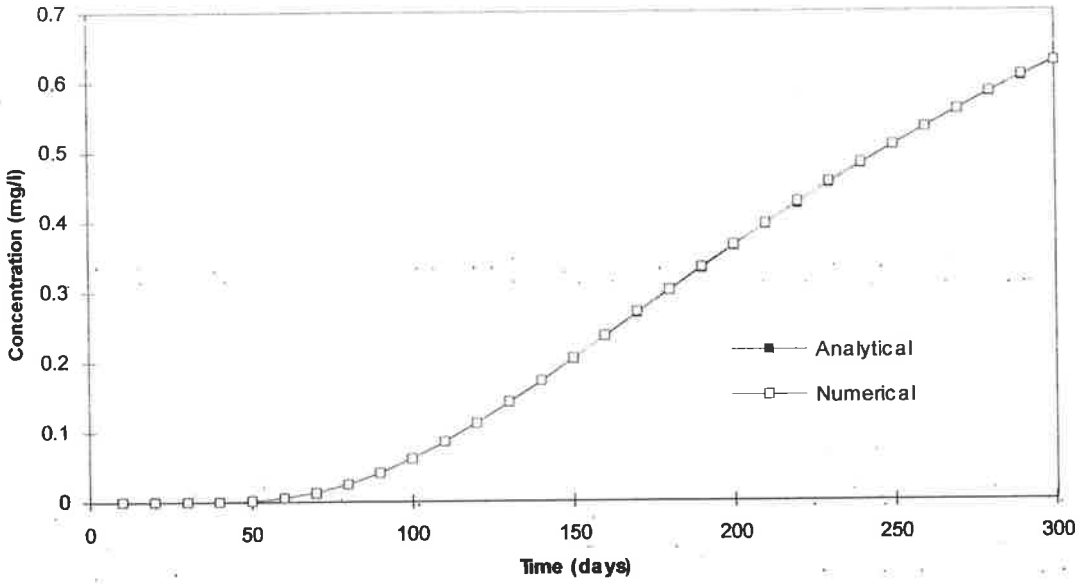



**Figure 6.15** 3-Dimensional model evaluation using breakthrough data at observation node 2 in layer 3

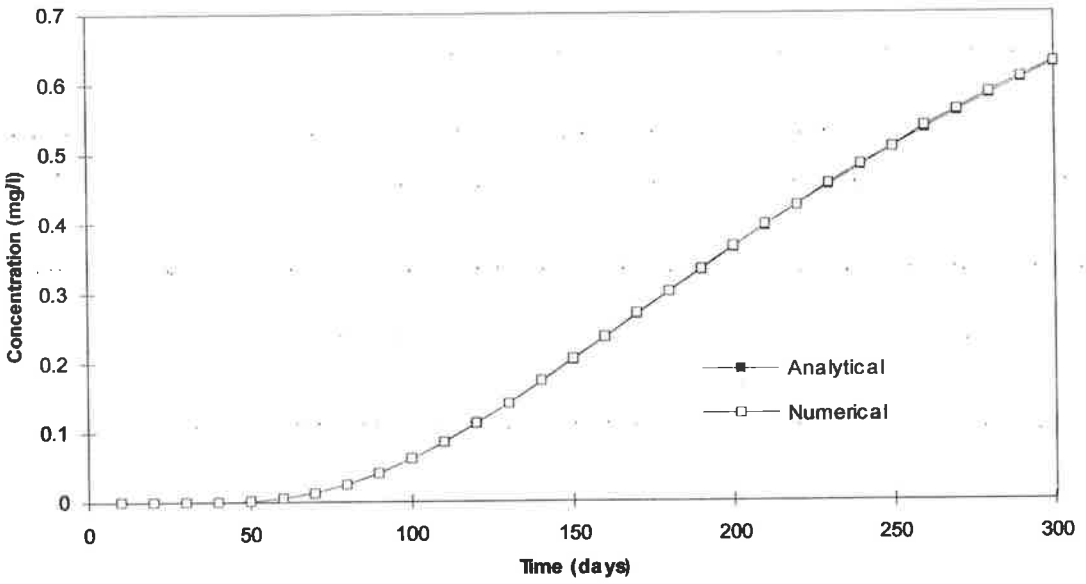



**Figure 6.16** 3-Dimensional model evaluation using breakthrough data at observation node 3 in layer 3

## 6.5 Summary

The application of the SCE technique has been extended to groundwater modelling using analytical models. The performance of the SCE technique with regard to analytical solute transport models have been tested and excellent results have been achieved. The technique was further tested together with a genetic algorithm method using the Theis analytical flow model and practical pumping field test data. In this regard, the performances of the evolutionary techniques were compared with a Gauss-Newton gradient based technique; in which the results of the evolutionary techniques matched favourably well with those of the traditional gradient-based Gauss-Newton method. The chapter concluded with the evaluation of two- and three-dimensional finite element solute transport models using some selected analytical models. The results of the numerical models were found to compare favourably well with those of the analytical for the simple cases of data considered. With the confidence that the developed models are giving the expected results, the analyses are extended to field scale scenarios through the use of numerical models. This is presented in chapter seven.

# Chapter 7

# Application to Field-Scale Problems

## 7.1 Introduction

The application of the inverse model of parameter identification to field-scale problems is presented in this chapter. In the previous chapter, this model was tested using analytical solute transport models with synthetic data and an analytical flow model with practical field pumping test data. In a field-scale analysis, analytical models lack the ability to handle nonhomogeneous and anisotropic problems. This limitation is usually surmounted in groundwater modelling through the use of numerical models. Numerical flow and solute transport models in both two- and three-dimensions are now embedded in the shuffled complex optimisation (SCE) model to solve the inverse problem of parameter identification. The following problems are considered in this chapter: (1) estimation of aquifer formation parameters under different flow conditions, (2) estimation of aquifer formation parameters using the transport model, and (3) a parametric analysis to study the weakness of the SCE inverse model.

## 7.2 Parameter Estimation by the Flow Model

In this context, $h_k^{sim}$ in equation (5.4) is obtained by solving the system of algebraic equations in (4.33) subject to the initial and boundary conditions in equations (4.5) to (4.7) for both the two- and three-dimensional models. In the two-dimensional mode, the parameters estimated are hydraulic conductivity in the x, y, and xy-directions and storage coefficient (ie. $k_{xx}$, $k_{yy}$, $k_{xy}$ $(= k_{yx})$, and $S$) while $k_{xx}$, $k_{yy}$, $k_{zz}$ and $S$ (where $k_{zz}$ is the vertical hydraulic conductivity) are estimated in the three-dimensional model. Parameters such as $k_{xx}$, $k_{yy}$, $k_{zz}$ and $S$ are continuous function of the spatial variables. For parameter identification purposes, a continuous function must be approximated by a finite dimensional form. Two methods that have been proposed in the literature are : (1) zonation method and (2) interpolation method. In this research, the method of zonation has been used for its simplicity. In the zonation method, the flow region is divided into a number of subregions called zones, and constant parameter value(s) is/are used to characterise each zone. In the finite element context, therefore, all elements falling within the same zone have the same parameter values. The dimension of parameterisation is represented by the product of the number of parameters under estimation and the number of zones into which the entire simulation region is subdivided. For example, if one seeks to estimate $k_{xx}$, $k_{yy}$, $k_{zz}$ and $S$ (four parameters) and the simulation region is parameterised into two zones, then the parameter dimension of the problem is eight .

Analyses are performed using both synthesised and corrupted synthesised data. The synthesised observed data is achieved by using known (or true) parameters to solve the forward problem in order to generate data for a number of observation points. The corrupted data is achieved by the random incorporation of noise in the synthesised data using the following expression:

$$h_i^{cd} = h_i^{sd}(1 \pm \omega * rand), \qquad i = 1,2,\ldots,nobs \tag{7.1}$$

where $h_i^{cd}$ is the generated corrupted data from the synthesised data $h_i^{sd}$; *rand* is a random number, *nobs* is the number of observation nodes, and $\omega$ is a fractional small parameter whose value must be reasonably selected in order to achieve sensible corrupted data. The rational behind the use of corrupted data is to test the strength of the SCE methodology with regard to field data which is known to contain observation errors or noise. The performance of the optimisation is evaluated by the computation of a parameter called the mean drawdown error. The mean drawdown error is the average of the absolute deviations of the predicted drawdown (using the final estimated parameters) from their respective observed values. In the case of the use of synthesised data the computed mean drawdown error must be quite close to or equal to zero for the final global optimum parameters. In the two-dimensional flow model, the analysis performed include parameter estimation in : (1) a homogeneous anisotropic aquifer, (2) an inhomogeneous and anisotropic aquifer with the axes of the hydraulic conductivity tensor aligned with those of the global axes, and (3) inhomogeneous and anisotropic with the axes of the conductivity tensor non-aligned with those of the global axes.

It is important to mention that modelling errors are not considered since the same mesh used to generate the data are used to determine the coefficients in the inverse problem. For this reason a uniform mesh was used; however a graded mesh could also have been used. In all analyses, the aquifer is assumed to be of the confined type. The results of these tests are presented and discussed in the sections that follow.

### 7.2.1 Homogeneous and Anisotropic Aquifer-Analysis 1

The simulation region whose parameters are to be estimated is shown in Figure 7.1 with its associated boundary conditions. An extraction well is located at the centre of the simulation region and observed data is synthesised at the four observation nodes shown in the figure. The observation and production wells are numbered according to the node numbers generated in the numerical model. The true parameters used in the synthesis of the observed data as well as the upper and lower limits of the parameters to be estimated are shown in Table 7.1. The simulation region is discretized into 14 nodes in the x-direction and 9 nodes in the y-direction in order to generate a total of 126 nodes and 104 elements. The nodal coordinates are generated using the following spatial increment scheme : $\Delta x = 40.0m$ and $\Delta y = 40.0m$. A constant time step of $\Delta t = 1.0$ days is used and a forward simulation is performed for a total of 10 time steps to obtain the synthesised data for each of the observation nodes. The generated drawdowns for both synthesised and corrupted data are shown in appendices 1a and 1b, respectively.

With regard to the SCE input parameters, two complexes - each containing a total of 9 sampling points - were required to solve this problem. The total number of population of points is equal to the product of the number of points in each complex and the number of complexes. Thus the entire number of initial population of points in the parameter search space was 18.

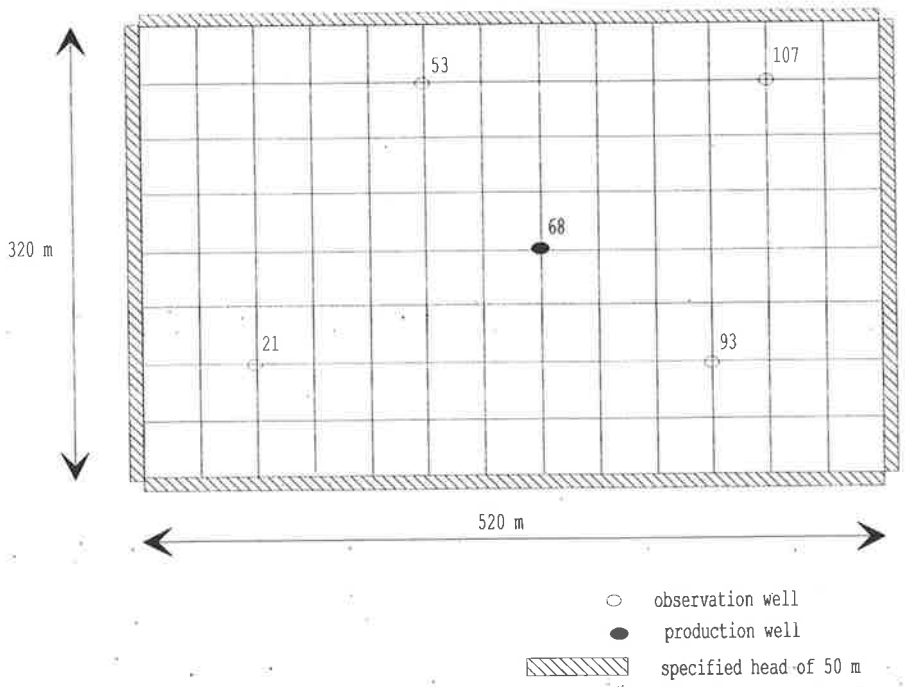



**Figure 7.1** A single-zone simulation region showing wells and boundary conditions

Intermediate parameters values required to repeatedly compute $h_k^{sim}$ by the numerical model for the evaluation of the objective function in equation (5.4) are generated in the optimisation model using the competitive complex evolution (CCE) in the SCE previously presented in chapter five. The parameters estimated in this analysis are *Kxx, Kyy, Kxy (=Kyx)*, and *S*. The final estimated parameters for the two analyses (with both synthesised and corrupted data) including their associated mean head errors are shown in Table 7.2.

**Table 7.1** True and boundary parameter values used in analysis 1

| *Kxx* [m/d] | *Kyy* [m/d] | *Kxy* [m/d] | *S* |
|---|---|---|---|
| True parameters used to generate observed data | | | |
| 50.0 | 35.0 | -2.50 | 0.0005 |
| | | | |
| Upper limits of parameters under estimation | | | |
| 200.00 | 200.00 | 50.00 | 1.0000 |
| | | | |
| Lower limits of parameters under estimation | | | |
| 0.00 | 0.00 | -50.00 | 0.0000 |

As it can be seen in Table 7.2, the final estimated parameters are almost the same as the true or expected parameters. This is indicated by the value of the mean drawdown error, which is the measure of the average absolute deviation of the simulated drawdowns from the observed drawdowns at the respective observation nodes. The results for the corrupted data is equally impressive. The nearness of the final estimated parameters, in the context of the corrupted data, to those of the true parameters indicate the potential strength of the SCE methodology in a real field-scale data analysis. It is appropriate to mention that because the aquifer is homogeneous, the need to parameterise the simulation region into zones was not necessary. In the subsequent applications, the technique is subjected to a region with more than one zone.

**Table 7.2** Summary results of analysis 1

| *Kxx* [m/d] | *Kyy* [m/d] | *Kxy* [m/d] | *S* |
|---|---|---|---|
| Expected or true parameters | | | |
| 50.0 | 35.0 | -2.50 | 0.0005 |
| | | | |
| Estimated parameters with synthetic data, mean head error = 1.43E-10 | | | |
| 50.000 | 35.000 | -2.499 | 0.4999E-03 |
| | | | |
| Estimated parameters with corrupted data, mean head error = 1.67E-08 | | | |
| 49.988 | 35.028 | -2.5059 | 0.50073E-03 |

### 7.2.2 Inhomogeneous and Anisotropic Aquifer with Kxy =0 -Analysis 2

In this analysis, the simulation region is parameterised into four zones with elements in a particular zone having the same values of aquifer formation parameters. Parameters *Kxy ( = Kyx)* are zero and hence not estimated in this analysis. In other words it is assumed that the global axes are aligned to those of the hydraulic conductivity tensor. The simulation region is shown in Figure 7.2. Once again both synthesised and corrupted data are used. The

simulation domain is a square region discretized into 11 nodes in both x- and y-directions. This results 121 nodes and 100 elements in the finite element network. The nodal coordinates of the discretized simulation region is generated using the following scheme: $\Delta x = 100.m$ and $\Delta y = 100.m$. Observation and production wells are numbered in accordance with the node numbering system generated in the numerical model. The true parameters used in each zone for the generation of the synthesised and corrupted observation data, including the boundary limits of the parameters under estimation are shown in Table 7.3. The resulting generated data (using the same time stepping scheme as analysis 1) are shown in appendices 2a and 2b.

5 complexes each containing 25 sampling points - and leading to a total of 125 sampling points in the entire parameter search space - were required by the SCE to solve the above problem. The total number of points in each complex (ie, 25 in this analysis) is obtained from the expression $2n+1$, where $n$ is the parameter dimensionality or the total number of parameters under estimation (ie, 12 (3 for each zone) in this analysis).

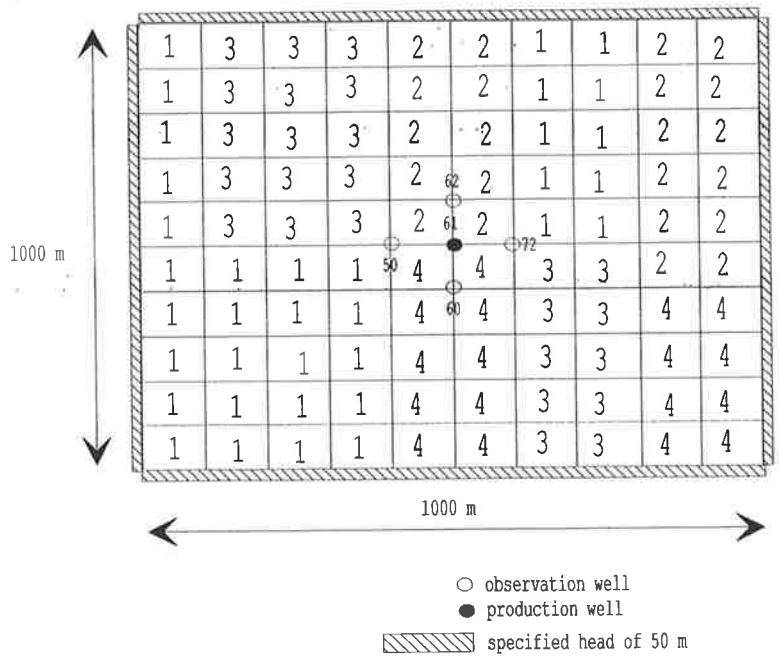



**Figure 7.2** A 4-zone simulation region showing zones, wells, and boundary conditions

The final estimated parameters for the synthesised and corrupted data are summarised in Table 7.4. In the case of the synthesised data, one can observe a very good agreement between the estimated and the expected parameters. This observation is supported by the small value of the mean drawdown error; which indicates that the predicted results obtained using the final estimated parameters are almost the same as the corresponding observed data shown in appendix 2a. The values of the final estimated data in the case of the corrupted data is equally good from the point of view of the fact that the data is assumed to be collected in the field (and therefore corrupted with noise). The present analysis has demonstrated that the SCE methodology has the potential to be used in simulation scenarios usually adopted in the context of the gradient-based techniques, ie, parameterisation of the simulation region into zones. In the final analysis of the two-dimensional flow model, the parameter identification model is applied to the estimation of the formation parameters for an inhomogeneous and anisotropic aquifer, where the global axes of the simulation region are not aligned with those of the hydraulic conductivity tensor (ie, $k_{xy} = k_{yx} \neq 0$).

**Table 7.3** True and boundary parameter values used in analysis 2

| | *Kxx* [m/d] | *Kyy* [m/d] | *S* |
|---|---|---|---|
| Zone | True parameters used to generate observed data | | |
| 1 | 60.00 | 50.00 | 0.001 |
| 2 | 45.00 | 35.00 | 0.002 |
| 3 | 30.00 | 20.00 | 0.003 |
| 4 | 20.00 | 10.00 | 0.004 |
| | | | |
| Zone | Upper limits of parameters under estimation | | |
| 1 | 100.00 | 100.00 | 1.0000 |
| 2 | 100.00 | 100.00 | 1.0000 |
| 3 | 100.00 | 100.00 | 1.0000 |
| 4 | 100.00 | 100.00 | 1.0000 |
| | | | |
| Zone | Lower limits of parameter under estimation | | |
| 1 | 0.00 | 0.00 | 0.0000 |
| 2 | 0.00 | 0.00 | 0.0000 |
| 3 | 0.00 | 0.00 | 0.0000 |
| 4 | 0.00 | 0.00 | 0.0000 |

**Table 7.4** Summary results of analysis 2

| | *Kxx* [m/d] | *Kyy* [m/d] | *S* |
|---|---|---|---|
| Zone | Expected or true parameters | | |
| 1 | 60.00 | 50.00 | 0.001 |
| 2 | 45.00 | 35.00 | 0.002 |
| 3 | 30.00 | 20.00 | 0.003 |
| 4 | 20.00 | 10.00 | 0.004 |
| | | | |
| Zone | Estimated parameters with synthetic data, mean head error = 3.751E-10 | | |
| 1 | 59.994 | 50.007 | 0.99967E-03 |
| 2 | 45.000 | 35.000 | 0.20000E-02 |
| 3 | 29.998 | 19.998 | 0.30002E-02 |
| 4 | 20.000 | 10.000 | 0.40001E-02 |
| | | | |
| Zone | Estimated parameters with corrupted data, mean head error = 1.093E-05 | | |
| 1 | 60.782 | 48.689 | 0.11059E-02 |
| 2 | 44.959 | 34.894 | 0.20019E-02 |
| 3 | 29.641 | 20.723 | 0.28807E-02 |
| 4 | 20.087 | 10.056 | 0.40073E-02 |

### 7.2.3 Inhomogeneous and Anisotropic Aquifer-Analysis 3

The simulation region, spatial and temporal discretization, and location of production and observation wells are the same as those used in analysis 2. As shown in Figure 7.3, the only difference here is the parameterisation of the region into three zones and the inclusion of anisotropic conditions (ie, $k_{xy} = k_{yx} \neq 0$) in the parameter estimation analysis. The observed drawdowns in the context of both the synthesised and the corrupted data are shown in appendices 3a and 3b, respectively. The parameters used in the generation of the observed data as wells as the upper and lower limits of the parameters under estimation are shown in Table 7.5. The number of complexes, number of points in each complex, and the total number of initialised points in the entire search space used in the SCE algorithm are respectively, 10, 25, and 250. The total number of parameters estimated is 12. It is interesting to note that these SCE parameters increase in magnitude as the problem becomes more complex and difficult to solve.

**Table 7.5** True and boundary parameter values used in analysis 3

| | *Kxx* [m/d] | *Kyy* [m/d] | *Kxy* [m/d] | *S* |
|---|---|---|---|---|
| Zone | True parameters used to generate observed data | | | |
| 1 | 40.00 | 30.00 | 1.50 | 0.002 |
| 2 | 30.00 | 20.00 | 1.00 | 0.003 |
| 3 | 50.00 | 35.00 | 1.75 | 0.001 |
| | | | | |
| Zone | Upper limits of parameters under estimation | | | |
| 1 | 150.00 | 150.00 | 5.00 | 1.0000 |
| 2 | 150.00 | 150.00 | 5.00 | 1.0000 |
| 3 | 150.00 | 150.00 | 5.00 | 1.0000 |
| | | | | |
| Zone | Lower limits of parameters under estimation | | | |
| 1 | 0.00 | 0.00 | 0.00 | 0.0000 |
| 2 | 0.00 | 0.00 | 0.00 | 0.0000 |
| 3 | 0.00 | 0.00 | 0.00 | 0.0000 |

The results of this analysis for both the synthesised and corrupted data after 182 and 100 cycles respectively, are shown in Table 7.6. The analyses with the synthetic data required a total of 62581 objective function evaluations to complete the analysis while in the use of the corrupted data, the analysis was completed the solution with 35144 objective function evaluations. Comparing the results of both analyses to the expected values in Table 7.6, a very good agreement can be observed. This is also supported by the values of the mean drawdown error for both the synthesised and the corrupted data. The values of the anisotropic hydraulic conductivity (*Kxy*=*Kyx*) parameters for the corrupted data appear to have deviated from their corresponding expected values. But considering the fact that only 4 observations wells are used against a problem of a parameter dimensionality of 12, and the relative magnitudes of *Kxy* (and *Kyx*) compared with *Kxx* and *Kyy*, the performance of SCE methodology in this regard may be considered as efficient.

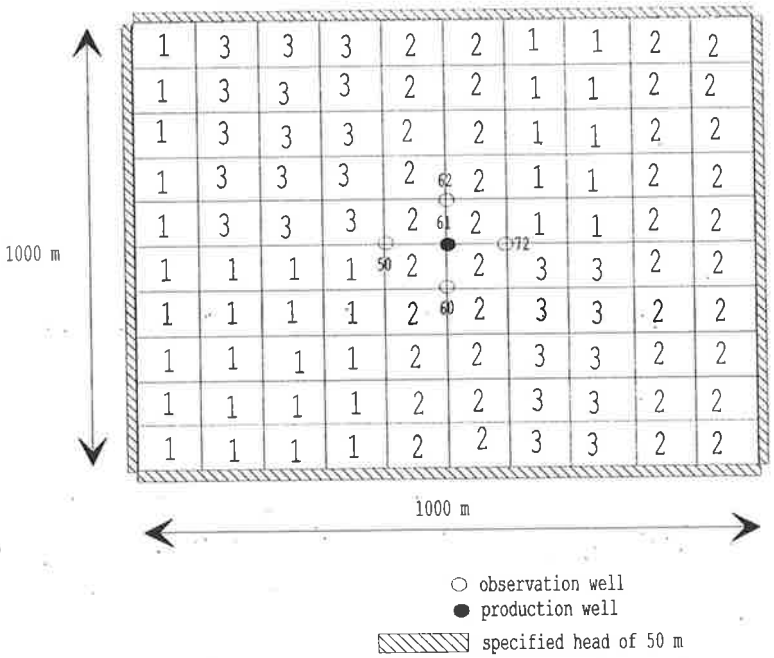



**Figure 7.3** A 3-zone simulation region showing zones, wells, and boundary conditions

**Table 7.6** Summary results of analysis 3

| | *Kxx* [m/d] | *Kyy* [m/d] | *Kxy* [m/d] | *S* |
|---|---|---|---|---|
| Zone | Expected or true parameters | | | |
| 1 | 40.00 | 30.00 | 1.50 | 0.002 |
| 2 | 30.00 | 20.00 | 1.00 | 0.003 |
| 3 | 50.00 | 35.00 | 1.75 | 0.001 |
| | | | | |
| Zone | Estimated parameters with synthesised data, mean drawdown error = 2.929E-10 | | | |
| 1 | 40.075 | 29.993 | 1.5777 | 0.20036E-02 |
| 2 | 30.000 | 20.000 | 0.9916 | 0.30000E-02 |
| 3 | 49.927 | 35.994 | 1.8454 | 0.99764E-03 |
| | | | | |
| Zone | Estimated parameters with corrupted data, mean drawdown error = 1.060E-05 | | | |
| 1 | 43.408 | 30.684 | 4.9974 | 0.21103E-02 |
| 2 | 30.022 | 19.978 | 2.2148 | 0.30082E-02 |
| 3 | 49.708 | 34.665 | 3.4501 | 0.99213E-03 |

Although they are not required to be the same, the deviation of the anisotropic parameters from those of the expected values in the case of the corrupted data is very significant. This indicates the extent of sensitivity of these parameters to small changes in drawdown values. But from such data assumed to be collected from the field, the primary objective of the analyst is the determination of the aquifer formation parameters that will

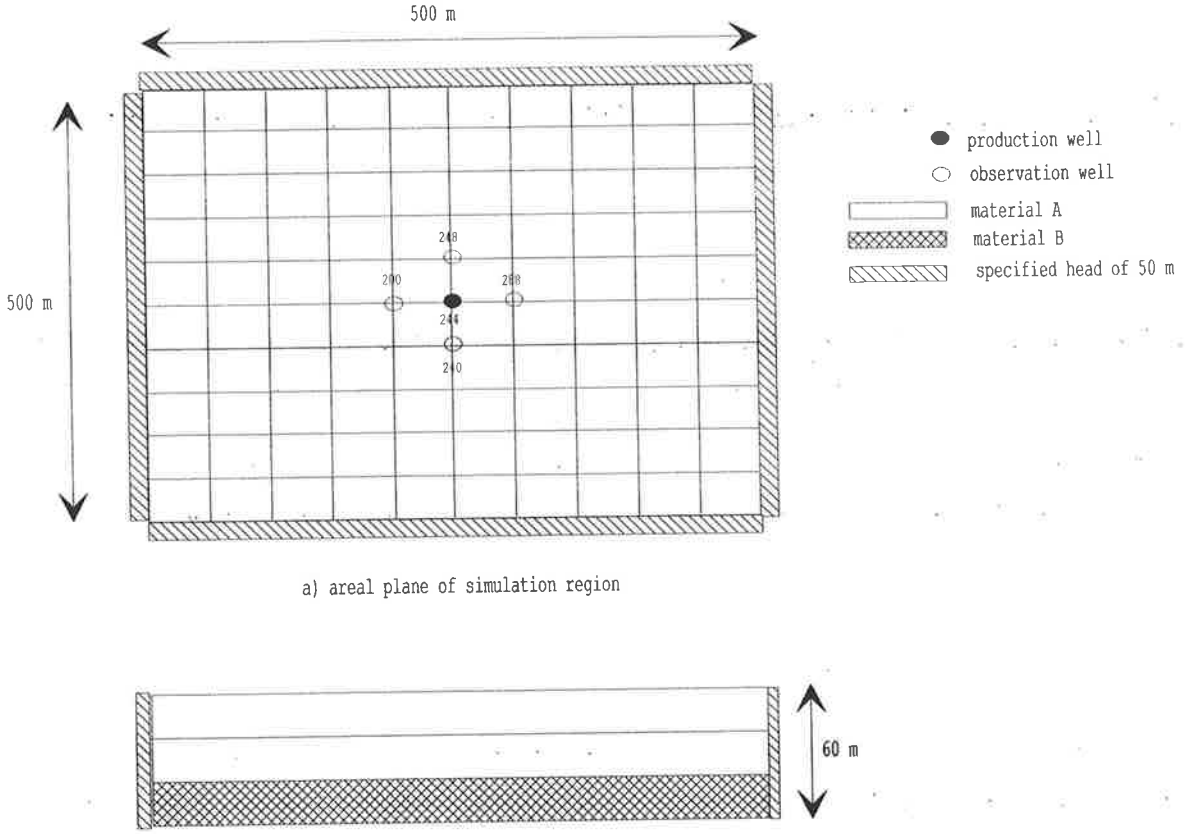
predict drawdowns to match the observed data as closely as possible. Hence, with a mean drawdown error value of 1.060E-05, any analyst will be convinced enough to consider the estimated parameters as true representatives of the aquifer formation from which the pumping test data was obtained. Nonetheless, the other parameters (*Kxx*, *Kyy*, and *S*) have compared favourably well with their respective true parameters. The performance of the SCE methodology, is tested against a three-dimensional flow model for the estimation of the parameters of an inhomogeneous aquifer in the following section.

## 7.2.4 3-D Inhomogeneous and Anisotropic Aquifer-Analysis 4

The three-dimensional simulation domain is shown in Figure 7.4. The region comprises a three-layered aquifer where the top and middle layers are of the same material A, and the bottom layer of material B. The region is therefore parameterised vertically into two zones and for each zone the parameters *Kxx*, *Kyy*, *Kzz*, and *S* are identified. This results in a parameter dimensionality of 8 for which data from four observation wells are used for the parameter estimation. The synthesised and the corrupted observed data are shown in appendices 4a and 4b, respectively. The true parameters used in the generation of the observed data are shown in Table 7.7 together with the upper and lower limits of the parameters under estimation.

In order to solve the forward problem, the simulation region is discretized into 11, 11, and 4 nodes in the x-, y-, and z-directions, respectively. This leads to a total 484 nodes and 300 elements. The numbering of the well nodes in Figure 7.4 is made in accordance with the node numbering system generated for the three-dimensional region in the numerical model. The coordinates of the nodes in the simulation region are generated using the following spatial increment scheme : $\Delta x = 50.m$, $\Delta y = 50.m$, and $\Delta z = 20.m$. The time stepping scheme is the same as that used in the previous analyses. With regard to the SCE

input parameters , the number of complexes, number of sample points in each complex, and the total number of points initialised in the entire search space are respectively, 10, 25, and 250.




a) areal plane of simulation region

b) vertical section of simulation domain

**Figure 7.4** Three-dimensional simulation region with wells and boundary conditions

The results of the final estimated parameters for both synthesised and corrupted data are shown in Table 7.8. The results for the synthesised data were achieved after a total of 104 cycles and 37814 objective function evaluations while those of the corrupted data were achieved with a total 88 cycles and 27184 objective function evaluations. Note that these figures are far lower than those obtained in analyses 3 in the two-dimensional case. This indicates that the SCE input parameters for the two-dimensional analyses (analysis 3) may have been over-selected. In particular, the SCE methodology is forced to loop through a large number of cycles and perform a large number of objective function evaluations if the

input SCE parameters are inadequate. As in the two-dimensional case, these results compare favourably well with the expected parameters. This observation is supported by the mean drawdown values also shown in the same table. This is a very significant achievement by the SCE methodology considering parameter dimensionality of the problem (8), the limited number of observation wells (4) and the scale of the problem (3-dimensional problem).

**Table 7.7** True and boundary parameter values used in analysis 4

| | *Kxx* [m/d] | *Kyy* [m/d] | *Kzz* [m/d] | *S* |
|---|---|---|---|---|
| Zone | True parameters used to generate observed data | | | |
| A | 50.00 | 30.00 | 15.00 | 0.001 |
| B | 40.00 | 20.00 | 10.00 | 0.003 |
| | | | | |
| Zone | Upper limits of parameters under estimation | | | |
| A | 100.00 | 100.00 | 100.00 | 1.0000 |
| B | 100.00 | 100.00 | 100.00 | 1.0000 |
| | | | | |
| Zone | Lower limits of parameters under estimation | | | |
| A | 0.00 | 0.00 | 0.00 | 0.00 |
| B | 0.00 | 0.00 | 0.00 | 0.00 |

**Table 7.8** Summary results of analysis 4

| | *Kxx* [m/d] | *Kyy* [m/d] | *Kzz* [m/d] | *S* |
|---|---|---|---|---|
| Zone | Expected or true parameters | | | |
| A | 50.00 | 30.00 | 15.00 | 0.001 |
| B | 40.00 | 20.00 | 10.00 | 0.003 |
| | | | | |
| Zone | Estimated parameters with synthesised data, mean drawdown error = 3.428E-10 | | | |
| A | 50.103 | 29.989 | 15.003 | 0.10002E-02 |
| B | 39.903 | 19.984 | 9.9833 | 0.29985E-02 |
| | | | | |
| Zone | Estimated parameters with corrupted data, mean drawdown error = 1.118E-05 | | | |
| A | 47.319 | 29.788 | 14.072 | 0.94916E-03 |
| B | 58.936 | 14.872 | 14.685 | 0.33295E-02 |

The question regarding the relationship between parameter dimesionality $L_D$, and the number of observation wells $N_0$, has been a very sensitive issue in the gradient-based parameter identification techniques. In fact, in the gradient-based context, all the three known techniques (influence coefficient method, sensitivity equation method, and variational method) available for the evaluation of the sensitivity matrix have limitations. *Yeh* [1986]

pointed out that instability owing to the use of any one of these techniques can be avoided (if the data contains noise) if the condition $N_0 > L_D$ is satisfied. Therefore, with regard to the parameter dimensionality and available number of observation wells relationship, the SCE technique appears to be superior to the gradient-based techniques because the former performs its search without need for computation of derivatives; making it more robust in terms of parameter sensitivity and interaction, and the extent of nonlinearity of the problem under consideration. It is interesting to note that with the exception of analysis 1 where $N_0 = L_D$, the SCE method has been able to solve all the other problems considered so far with $N_0 < L_D$.

## 7.3 Parameter Estimation- Transport Model

Application of the SCE methodology to parameter identification in a solute transport numerical model is similar to the case of the analytical models (presented in chapter six) except for two major differences : (i) evaluation of the objective function in equation (5.4) requires the solution of the system of algebraic equations in (4.38) to obtain $c_k^{sim}$ and (ii) the simulation region is allowed to be parameterised into zones to account for nonhomogeneity of the aquifer. In the context of nonhomogeneous aquifers, the simulation region is subdivided into zones wherein all elements falling into the same zone have common values of aquifer formation parameters. In the solute transport context, the parameters estimated by the inverse model are the longitudinal dispersivity ($\alpha_L$), the transverse dispersivity ($\alpha_T$), and the aquifer porosity ($\phi$) for homogeneous and nonhomogeneous aquifers.

To demonstrate the potential strength of the SCE technique in solving practical field-scale problems, the synthesised data is further corrupted with random noise to emulate field data. A second simulation is then performed with the corrupted data as it was done in the

flow model. Synthetic data are obtained by using known (or true) aquifer parameters to generate the observed data $c_i^{obs}$ through the solution of the forward problem only. Subsequently, the corrupted data $c_i^{cd}$, are obtained from the expression:

$$c_i^{cd} = c_i^{obs}(1 \pm \omega * rand), \qquad i = 1,2,....nobs \tag{7.2}$$

where *rand*, $\omega$, and *nobs* have meanings similar to those defined in equation (7.1). The mean concentration error (mcerr) is evaluated as a measure of the efficiency of the solution. The two numerical problems that are used to test the strength of the SCE in the two-dimensional context are the parameter estimation of a : (1) homogeneous aquifer, and (2) nonhomogeneous aquifer. The results of these tests are presented in the following sections.

### 7.3.1 Homogeneous Aquifer-Analysis 5

The two-dimensional region of the homogenous aquifer whose parameters are under investigation is shown in Figure 7.5. The simulation region is discretized into 9 nodes along the y-axis and 15 nodes along the x-axis; resulting in a total of 135 nodes and 112 elements in the entire finite element network. The nodal coordinates of the discretized region are computed using the following spatial increment scheme : $\Delta x = 25.0m$ and $\Delta y = 25.0m$. Using a constant time step of $\Delta t = 10.0$ days, a forward simulation is performed for a total of 10 time steps to generate the synthesised and corrupted data for each of the observation nodes. The synthesised and corrupted data are shown in appendices 5a and 5b, respectively. In the SCE model, only 2 complexes are required for the analysis. Each of these complexes has 7 sample points leading to a population of 14 points initialised in the entire search space. The other input parameters required by the SCE are the lower and upper bounds of the

parameters under estimation. The values of these limits in addition to the true parameters used to generate the observed data are shown in Table 7.9.

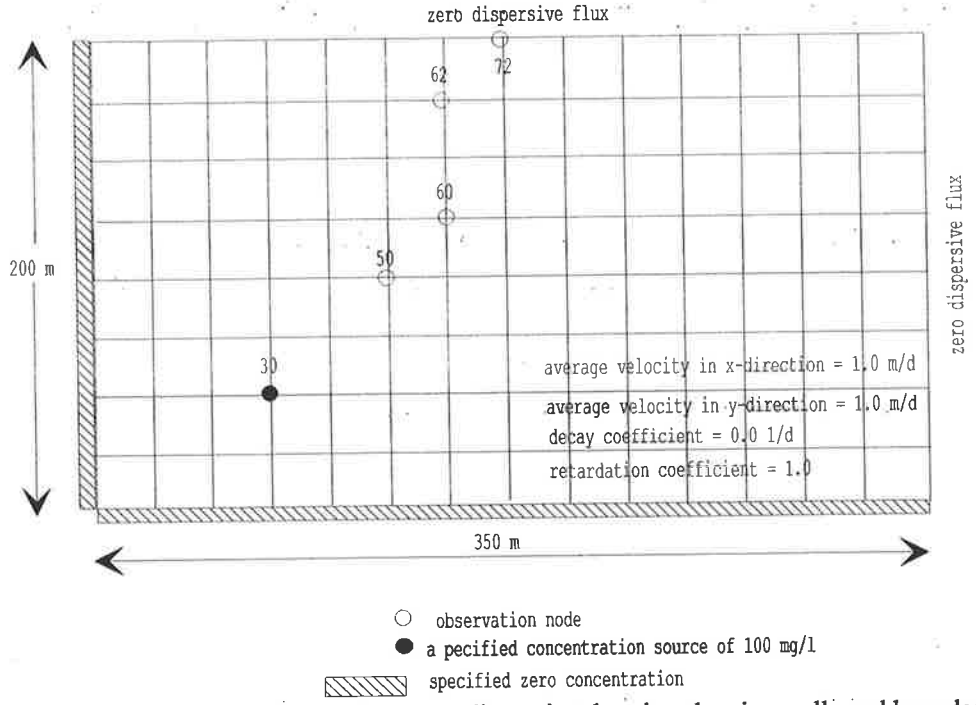



**Figure 7.5** Homogeneous two-dimensional region showing wells and boundary conditions

**Table 7.9** True and boundary parameter values used in analysis 5

| $\alpha_L$ [m] | $\alpha_T$ [m] | $\phi$ |
|---|---|---|
| True parameters used to generate observed data | | |
| 50.00 | 30.00 | 0.1500 |
| | | |
| Upper limits of parameters under estimation | | |
| 200.00 | 200.00 | 1.00 |
| | | |
| Lower limits of parameters under estimation | | |
| 0.00 | 0.00 | 0.00 |

**Table 7.10** Summary results of analysis 5

| $\alpha_L$ [m] | $\alpha_T$ [m] | $\phi$ |
|---|---|---|
| Expected or true parameters | | |
| 50.00 | 30.00 | 0.1500 |
| | | |
| Estimated parameters with synthetic data, mcerr = 1.040E-10 | | |
| 50.000 | 30.0000 | 0.1500E+00 |
| | | |
| Estimated parameters with corrupted data, mcerr = 1.700E-02 | | |
| 50.483 | 30.063 | 0.1505E+00 |

The final estimated values of the parameters including their expected values are shown in Table 7.10 for both synthesised and corrupted data. These values appear to be in a good agreement with the expected parameters in the context of both the synthesised and corrupted data. In the context of the synthesised data, the SCE estimated parameters whose values are the same as the expected values. One should therefore expect the mean concentration error value for this analysis to be zero. This is not the case in this analysis because the results of the final estimated parameters have been printed to only four decimal places. However, considering the nearness of the estimated parameters to the expected parameters, it suffices to say that the SCE search technique is robust and efficient.

From the corrupted data perspective, the values of the final estimated parameters are not expected to be too close to the true values because the observed data is corrupted. However, the true parameters could serve as a standard measure to determine how reasonable the parameters estimated with the corrupted data are. This is because the corrupted data are minor random deviations from the synthesised data. With this in mind, one can observe from Table 7.10 that the final estimated parameters with regard to the corrupted data are sensible. Compared to the flow models, the mean concentration error appears to be very large (ie. 1.70E-02) although the final estimated parameters are quite close to the expected parameters except for the longitudinal dispersivity value ($\alpha_L$). The explains the

extent of sensitivity of the solute transport parameters to small changes in the concentration data compared to the flow parameters.

### 7.3.2 Nonhomogeneous Aquifer-Analysis 6

The simulation region for this problem, the spatial discretization, boundary conditions, and locations of observation wells are the same as those for the analysis 1. The time stepping scheme is set at $\Delta t = 5.0$ days and the numerical forward simulation is performed for a total of ten time steps to generate the synthesised and corrupted data shown in appendices 6a and 6b, respectively. As it can be seen in Figure 7.6, the major difference between the present and previous analysis is the parameterisation of the region into four zones each with its distinct parameter values of $\alpha_L$, $\alpha_T$, and $\phi$. The parameter dimensions is 12 (the number of parameters under estimation in each zone multiplied by the number of zones into which the entire region is parameterised) and 4 observation nodes are used to identify the parameters in each zone. It is noted here that $L_D > N_0$ in this analysis (ie. $L_D = 12$, $N_0 = 4$). The true parameters used in the generation of synthesised data (and subsequently corrupted data) including the upper and lower limits of the parameters under estimation are shown in Table 7.11.

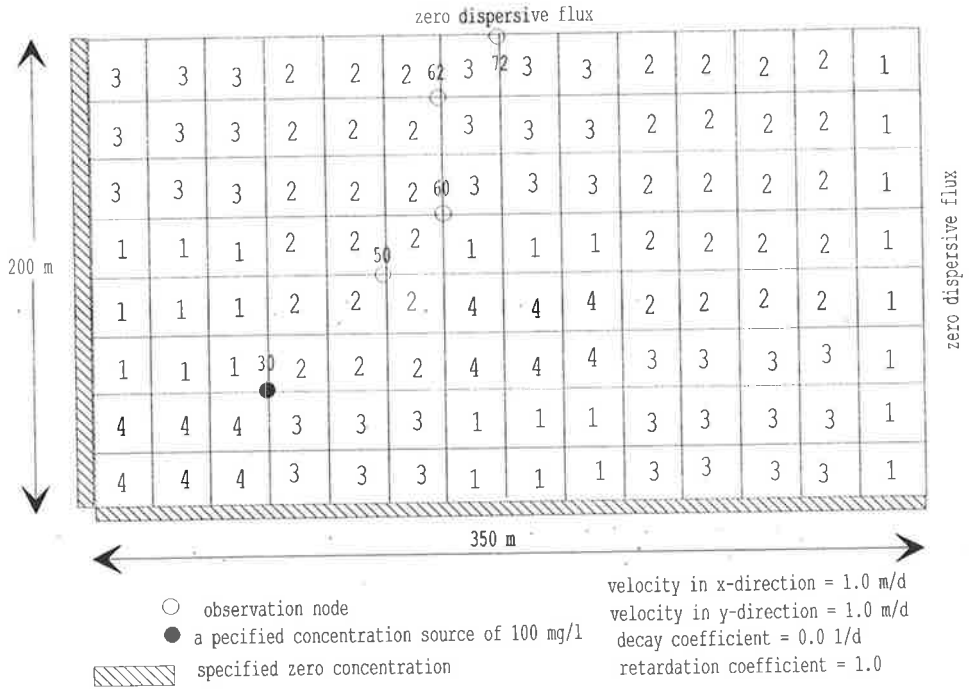



**Figure 7.6** A 4-zone simulation region showing wells and boundary conditions

Because of the complexity of the problem with regard to the number of zones, the search space is partitioned into 10 complexes. Each complex has a sample size of 25 members; leading to a population size of 250 points in the entire search space. The final results of the analyses with regard to both synthesised and corrupted data are shown in Table 7.12. From the results of this table, one can observe a very good agreement between the expected and the estimated parameters in the context of the synthesised data despite the fact that $L_D > N_0$. This indicates the capability of the SCE technique in handling simulation scenarios usually adopted in the traditional gradient-based techniques (ie., reduction of continuous parameters to finite dimensional form via zonation) . The wide range between the upper and lower limits used as a starting base for the SCE model and the fact that the parameter dimensionality is far greater than available number of observations, supports the robustness of the technique in its search procedures. Considering the values of the true parameters in Table 7.12, the estimated parameters in the context of the corrupted data are very reasonable. The mean concentration error (mcerr) of 6.664E-06 indicates the potential

strength of the technique in the handling of parameter instability in noisy data and under conditions where the parameter dimensionality of the problem is greater than the available number of observation nodes or wells.

**Table 7.11** True and boundary parameter values used in analysis 6

| | $\alpha_L$ [m] | $\alpha_T$ [m] | $\phi$ |
|---|---|---|---|
| Zone | True parameters used to generate observed data | | |
| 1 | 150.00 | 120.00 | 0.2500 |
| 2 | 135.00 | 105.00 | 0.1500 |
| 3 | 125.00 | 100.00 | 0.3500 |
| 4 | 145.00 | 115.00 | 0.4500 |
| | | | |
| Zone | Upper limits of parameters under estimation | | |
| 1 | 250.00 | 250.00 | 1.0000 |
| 2 | 250.00 | 250.00 | 1.0000 |
| 3 | 250.00 | 250.00 | 1.0000 |
| 4 | 250.00 | 250.00 | 1.0000 |
| | | | |
| Zone | Lower limits of parameters under estimation | | |
| 1 | 0.00 | 0.00 | 0.00 |
| 2 | 0.00 | 0.00 | 0.00 |
| 3 | 0.00 | 0.00 | 0.00 |
| 4 | 0.00 | 0.00 | 0.00 |

**Table 7.12** Summary results of analysis 6

| | $\alpha_L$ [m] | $\alpha_T$ [m] | $\phi$ |
|---|---|---|---|
| Zone | Expected or true parameter | | |
| 1 | 150.00 | 120.00 | 0.2500 |
| 2 | 135.00 | 105.00 | 0.1500 |
| 3 | 125.00 | 100.00 | 0.3500 |
| 4 | 145.00 | 115.00 | 0.4500 |
| | | | |
| Zone | Estimated parameter values with synthesised data , mcerr = 2.471E-10 | | |
| 1 | 150.01 | 120.00 | 0.25001 |
| 2 | 134.99 | 104.99 | 0.14999 |
| 3 | 125.00 | 99.998 | 0.34999 |
| 4 | 145.09 | 115.03 | 0.45016 |
| | | | |
| Zone | Estimated parameter values with corrupted data , mcerr = 6.664E-06 | | |
| 1 | 150.04 | 119.81 | 0.24978 |
| 2 | 136.80 | 106.23 | 0.15195 |
| 3 | 124.42 | 99.748 | 0.34767 |
| 4 | 135.15 | 110.72 | 0.43046 |

Compared to analysis 5, the mean concentration error of 6.664E-06 portrays a very good performance of the SCE model for zonal transport problems. Perhaps the difference between the present analysis and analysis 5 may be due to the large number of zones that calls for the use of large values of complexes, and hence a greater number of population of points initialised in the entire search space. The effect of the number of complexes on the values of the parameters estimated is considered in section 7.5.

The two problems handled in the three-dimensional scenario are (1) a simple nonhomogeneous aquifer, and (2) a 'tricky' nonhomogeneous aquifer. The 'tricky' nonhomogeneous aquifer is used to test the robustness and versatility of the SCE search procedures in a three-dimensional numerical model.

### 7.3.3 A Simple 3-D Nonhomogeneous Aquifer - Analysis 7

The three-dimensional simulation region is shown in Figure 7.7. The aquifer region comprises three distinct layers each of which has its unique material properties. This leads to the recognition that elements within the same layer have common material properties. Considering the fact that $\alpha_L$, $\alpha_T$, and $\phi$ are to be estimated for each layer, the parameter dimensionality is 9 and the available number of observation wells are 4.

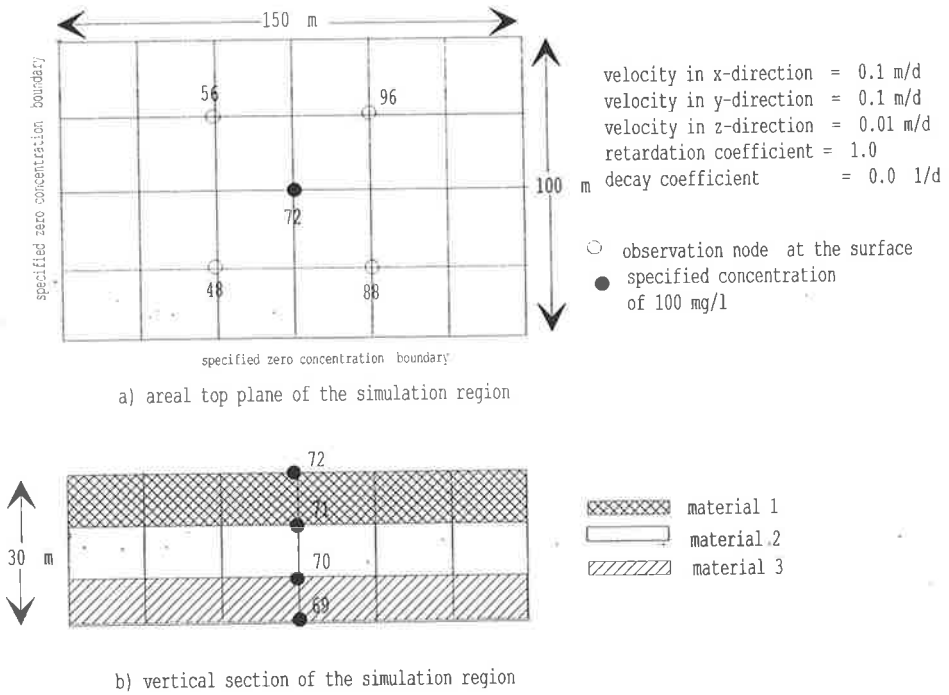



**Figure 7.7** Three-dimensional simulation region showing wells and boundary conditions

The simulation region is discretized into 7 nodes in the x-direction, 5 nodes in the y-direction, and 4 nodes in the z-direction. This leads to a total of 140 nodes and 72 elements in the entire finite element network. The nodal coordinates are generated using the following spatial increment scheme : $\Delta x = \Delta y = 25m$, and $\Delta z = 10m$. A constant time step size of $\Delta t = 20$ days is used and the numerical forward problem is performed for 10 times steps to generate the observation data for the nodes shown in Figure 7.7. The specified concentration nodes and observation wells shown in Figure 7.7 are numbered in accordance with the node numbers generated in the finite element network. The true parameter values of each layer used in the generation of the synthesised and corrupted data (see appendices 7a and 7b), including the lower and upper limits of the parameters under estimation are shown in Table 7.13. In the SCE model, 10 complexes, each containing 19 sampled points is required to solve the problem. This results in a total population of 190 points initialised in the search space. The results of the analysis for both the synthesised and corrupted data are shown in Table 7.14.

**Table 7.13** True and boundary parameter values used in analysis 7

| | $\alpha_L$ [m] | $\alpha_T$ [m] | $\phi$ |
|---|---|---|---|
| Zone | True parameters used to generate observed data | | |
| 1 | 85.00 | 50.00 | 0.2500 |
| 2 | 100.00 | 60.00 | 0.3500 |
| 3 | 75.00 | 45.00 | 0.1500 |
| | | | |
| Zone | Upper limits of parameters under estimation | | |
| 1 | 250.00 | 250.00 | 1.0000 |
| 2 | 250.00 | 250.00 | 1.0000 |
| 3 | 250.00 | 250.00 | 1.0000 |
| | | | |
| Zone | Lower limits of parameters under estimation | | |
| 1 | 0.00 | 0.00 | 0.00 |
| 2 | 0.00 | 0.00 | 0.00 |
| 3 | 0.00 | 0.00 | 0.00 |

One can observe that the estimated parameters in the context of both the synthesised and the corrupted data agree very well with the expected parameters. This again indicates the strength of the SCE technique in handling the inverse problem of parameter identification in a three-dimensional transport model and in a particular case where the parameter dimensionality (9) is far greater than the number of observations (4). A situation like this has been documented to create problems of parameter instability in context of the traditional gradient-based techniques [*Yeh*, 1986].

**Table 7.14** Summary results of analysis 7

| | $\alpha_L$ [m] | $\alpha_T$ [m] | $\phi$ |
|---|---|---|---|
| Zone | Expected or true parameters | | |
| 1 | 85.00 | 50.00 | 0.2500 |
| 2 | 100.00 | 60.00 | 0.3500 |
| 3 | 75.00 | 45.00 | 0.1500 |
| | | | |
| Zone | Estimated parameter values with synthesised data, mcerr = 1.569E-06 | | |
| 1 | 84.600 | 49.643 | 0.25081 |
| 2 | 100.00 | 60.069 | 0.34954 |
| 3 | 75.013 | 45.010 | 0.15022 |
| | | | |
| Zone | Estimated parameter values with corrupted data, mcerr = 2.221E-04 | | |
| 1 | 88.790 | 49.789 | 0.25128 |
| 2 | 99.814 | 57.928 | 0.34509 |
| 3 | 72.017 | 43.011 | 0.15022 |

## 7.3.4 The 3-D 'tricky' Nonhomogeneous Aquifer - Analysis 8

The three-dimensional simulation region is shown in Figure 7.8. As it can been seen in the figure, layers 1 and 3 have the same aquifer material properties. However, this issue is hidden from the SCE algorithm by identifying layer three with a unique material identification number of 3 (instead of 1). The material identification numbers are used to parameterise the region into zones. Elements in the same zone have common aquifer material properties and hence are identified by the same material number. The objective of identifying the third layer with a different material identification number is to investigate whether the SCE is robust enough to estimate the same parameters for layers 1 and 3. The simulation region is discretized to contain 9 nodes in the x-direction, 7 nodes in the y-direction, and 4-nodes in the z-direction This leads to a total of 252 nodes and 144 elements in the entire finite element network. The spatial discretization parameters used in the evaluation of the nodal coordinates, and time stepping scheme are the same as those used in analysis 7.

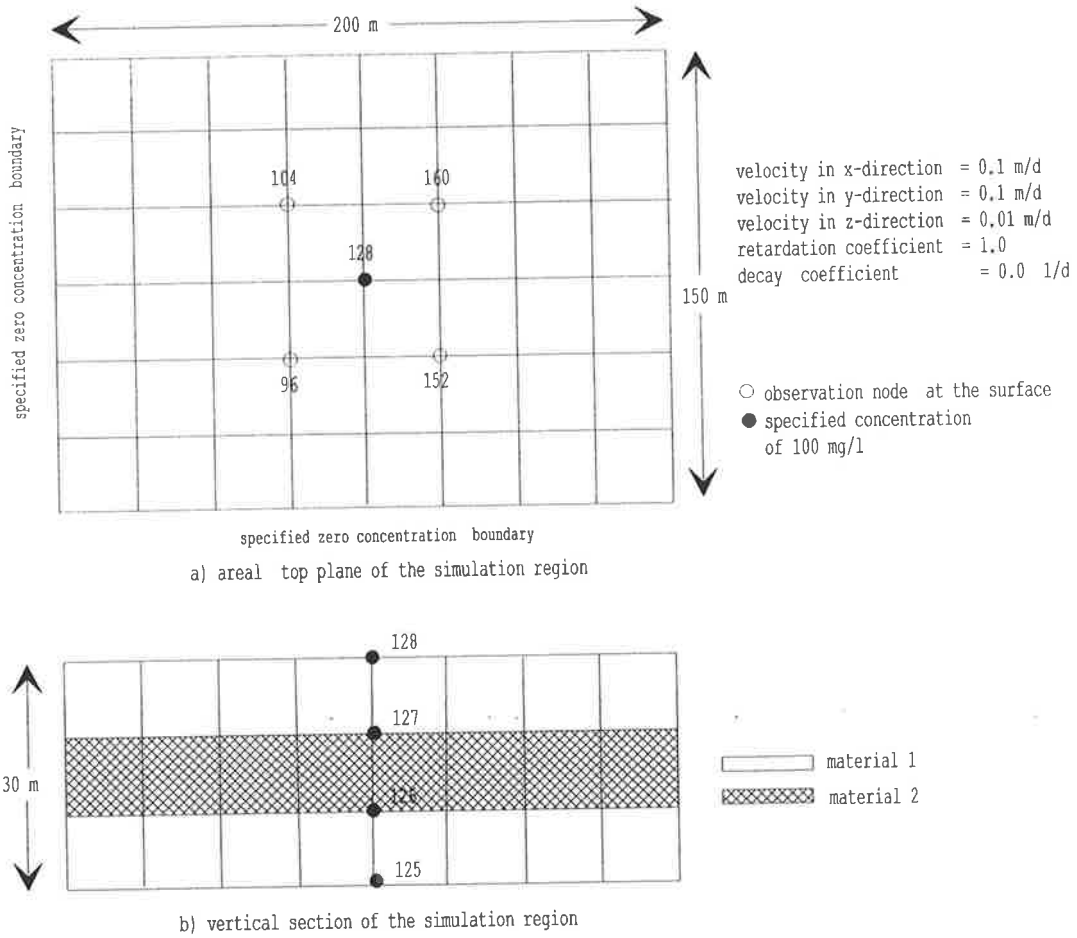



**Figure 7.8** Three-dimensional simulation region showing wells and boundary conditions

The true parameters used in the evaluation of the synthesised and corrupted data, as well as the lower and upper limits of the parameters under estimation are shown Table 7.15. The synthesised and corrupted data generated for this analysis are shown in appendices 8a and 8b. It must be noted in Table 7.15 that the upper limits of the material zone 3 has been given different values from the other two layers to further conceal the fact that layers 1 and 3 have the same material properties. Although generation of parameter values are done randomly (and hence similarities of limits are not important), the use of different upper limits is applied to ensure that any bias towards the achievement of the same parameter values for layers 1 and 3 is removed from the analysis.

**Table 7.15** True and boundary parameter values used in analysis 8

| | $\alpha_L$ [m] | $\alpha_T$ [m] | $\phi$ |
|---|---|---|---|
| Zone | True parameters used to generate observed data | | |
| 1 | 80.00 | 50.00 | 0.2500 |
| 2 | 100.00 | 60.00 | 0.3500 |
| 3 | 80.00 | 50.00 | 0.2500 |
| | | | |
| Zone | Upper limits of parameters under estimation | | |
| 1 | 250.00 | 250.00 | 1.0000 |
| 2 | 250.00 | 250.00 | 1.0000 |
| 3 | 200.00 | 200.00 | 0.8000 |
| | | | |
| Zone | Lower limits of parameters under estimation | | |
| 1 | 0.00 | 0.00 | 0.00 |
| 2 | 0.00 | 0.00 | 0.00 |
| 3 | 0.00 | 0.00 | 0.00 |

As in analysis 7, 10 complexes , with 19 points in each complex, are required for a successful completion of the analysis. The results of the analysis for both the synthesised and corrupted data are shown in Table 7.16. One can observe that under such difficult conditions, the SCE methodology has not only been able to estimate the correct parameters but also to reveal the fact that the material properties of layers 1 and 3 are the same in the context of the synthesised observed data. Compared with the values of the expected parameters, the results of the estimated parameters with the corrupted data are also equally impressive. These excellent results obtained in the present analysis is also supported by the values of the mean concentration errors (mcerr) also shown in the Table 7.16. This particular analysis has again confirmed the robustness, effectiveness, and efficiency of the SCE search scheme. It must be emphasised that the use of the same parameter limit values is not a requirement since initial and intermediate computation of parameters required for evaluation of the objective function (where necessary) are performed stochastically (ie. on a random basis). However, common values have been used in almost all problems that require the subdivision of the simulation region into zones in order to demonstrate the effectiveness and robustness of the SCE search procedures in cases where the parameters being sought for have different magnitudes for each zone.

**Table 7.16** Summary results of analysis 8

| | $\alpha_L$ [m] | $\alpha_T$ [m] | $\phi$ |
|---|---|---|---|
| Zone | Expected parameters | | |
| 1 | 80.00 | 50.00 | 0.2500 |
| 2 | 100.00 | 60.00 | 0.3500 |
| 3 | 80.00 | 50.00 | 0.2500 |
| | | | |
| Zone | Estimated parameter values with synthesised data, mcerr = 3.052E-10 | | |
| 1 | 79.981 | 49.986 | 0.24993 |
| 2 | 100.05 | 60.028 | 0.35017 |
| 3 | 79.993 | 49.996 | 0.24998 |
| | | | |
| Zone | Estimated parameter values with corrupted data, mcerr = 8.961E-05 | | |
| 1 | 81.005 | 50.176 | 0.24938 |
| 2 | 99.183 | 59.833 | 0.35275 |
| 3 | 79.935 | 49.901 | 0.24903 |

## 7.5 Where the SCE Fails

A number of flow and solute transport examples have been used in the previous sections to demonstrate - in terms of numerical modelling - the performance and efficiency of the SCE optimisation method of the inverse problem of parameter identification. In this section, particular attention is given to the identification of the weakness of the SCE optimisation technique. In this regard, it is appropriate to demonstrate with some examples, for situations where the SCE methodology is likely to fail. This objective is achieved through a parametric study of the sensitivity of the basic input parameter to the SCE model - the number of complexes $p$.

If the number of parameters under estimation $n$ is known, such input parameters as the number of points in a complex $m$, the number of points in subcomplex $q$, and the number of evolution steps taken by each complex $\beta$, are evaluated as [*Duan et al.*, 1994]:

$$
\begin{aligned}
m &= 2n+1 \\
q &= n+1 \\
\beta &= m
\end{aligned}
\qquad (7.3)
$$

Therefore the only input parameter whose value requires the judgment of the analyst is the number of complexes $p$. Using the data for analysis 3 of the flow model a series of 13 runs are performed, each time changing the value of $p$, to determine the performance of the SCE technique. The basic SCE input parameters used in this parametric for the entire 13 runs is shown in Table 7.17.

**Table 7.17** SCE input parameters used in the parametric study

| *par* | run 1 | run 2 | run 3 | run 4 | run 5 | run 6 | run 7 | run 8 | run 9 | run 10 | run 11 | run 12 | run 13 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| *p* | 3 | 4 | 5 | 6 | 8 | 10 | 12 | 15 | 20 | 25 | 30 | 35 | 40 |
| *m* | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 25 |
| *q* | 13 | 13 | 13 | 13 | 13 | 13 | 13 | 13 | 13 | 13 | 13 | 13 | 13 |
| $\beta$ | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 25 |
| *ts* | 75 | 100 | 125 | 150 | 200 | 250 | 300 | 375 | 500 | 625 | 750 | 875 | 1000 |

In Table 7.17, *par* stands for parameter and *ts* for total number of population of points initialised in the search space. The total number of population of points *ts*, is obtained by multiplying the number of complexes $p$ set for each run by the corresponding number of points in a complex, $m$. Since the number of parameters under estimation $n$, remains constant at 12, the SCE input parameter values $m$, $q$, and $\beta$ remain the same for all the 13 runs performed in the sensitivity analyses. The lower and upper limits of the parameters under estimation, including the expected parameters for each zone are reproduced in Table 7.18. With all the input parameters set, the objective of the sensitivity analysis is to study the efficiency of the SCE methodology in estimating the parameters under consideration as the number of complexes $p$, vary from as low as 3 to as high as 40.

The results of the estimated parameters including the efficiency of performance *eff*, for each run are shown in Tables 7.19a to 7.19c. The measure of efficiency of the SCE for

each run is evaluated by computing the average deviations of the predicted results - using the final estimated parameters - from the synthesised data. The synthesised data used in this parametric study are the same as those used in analysis 3 (appendix 3a). For efficient results, the value of *eff* must be as close as possible to zero. In other words the larger the value of *eff*, the poorer the values of the final estimated parameters.

The summary results shown in Table 7.19a indicate that none of the number of complexes set for the problems (ie, with $p$ = 3, 4, 5, 6, and 8) could generate final parameters as close as possible to the true or expected parameters in Table 7.18. However, it is interesting to observe from Table 7.19a that the efficiency of the solution improves as the number of complexes increase. From Table 7.17 it can be observed that the total number of initialised population points , *ts* , in the sample space increase as the number of complexes increase. It may thus be concluded that the ability of the SCE to solve a problem successfully depends on the number of sample points initialised in the search space. For $p$ = 3, 4, 5, 6, and 8, the total number of population points (*ts* = 75, 100, 125, 150, and 200) initialised in the search space are inadequate for the SCE to optimise from. The sample space may therefore be considered as 'sparsely populated ' for these number of complexes. The fact that the solution improves from one run to the next as the number of complexes (and hence the total number of initialised points, *ts*) increase clearly confirms the rationale behind the assertion that the inadequate total number of initialised population points in the search space may be responsible for the inefficient performance of the SCE.

On the other hand, one can observe that the efficiency of solution in Tables 7.19b and 7.19c converge to the same values for the number of complexes considered in these runs. Comparing the estimated parameters for each of the runs in these two tables to the expected parameters in Table 7.18, it can be observed that the estimated parameters agree favourably well with the expected parameters for all the number of complexes set for these runs. It also interesting to note that the level of performance of the SCE for each run is the same for all the results in these two tables. The revelation here implies that the use of a very large number

of complexes may yield the appropriate results but the solution may not be cost effective since it will require a greater number of objective function evaluations and hence a considerable length of time to arrive at the final optimum parameters. For these solutions Table 7.20 indicates that the best solution with respect to cost effectiveness is RUN 5 since the problem in question is solved with a larger number of cycles but smaller number of objective function evaluations.

In general the plot of the graph of efficiency of the number of complexes used in a problem (see Figure 7.9) indicates that the SCE's solution is likely to fail if the number of complexes used - and hence the population of points in the search space - is inadequate. However, the use of unreasonably high number of complexes only results in a solution that is rather expensive with regard to computational time. In this parametric study, it may be concluded that the optimal number of complexes required for an efficient and cost-effective solution is when $p$ = 10. This is because the solution process requires a large number of cycles but small number of objective function evaluations as compared to the other solutions in Tables 7.19b and 7.19c. Experience in this work has however shown that a more efficient and cost-effective solution can be achieved if the optimum number of complexes or communities $p_{opt}$, is selected such that: $n-2 \le p_{opt} \le n+2$; where $n$ is the number of parameters under estimation.

**Table 7.18** True parameters with their corresponding upper and lower limits

| | *Kxx* [m/d] | *Kyy* [m/d] | *Kxy* [m/d] | *S* |
|---|---|---|---|---|
| Zone | True parameters used to generate observed data | | | |
| 1 | 40.00 | 30.00 | 1.50 | 0.002 |
| 2 | 30.00 | 20.00 | 1.00 | 0.003 |
| 3 | 50.00 | 35.00 | 1.75 | 0.001 |
| | | | | |
| Zone | Upper limits of parameters under estimation | | | |
| 1 | 150.00 | 150.00 | 5.00 | 1.0000 |
| 2 | 150.00 | 150.00 | 5.00 | 1.0000 |
| 3 | 150.00 | 150.00 | 5.00 | 1.0000 |
| | | | | |
| Zone | Lower limits of parameters under estimation | | | |
| 1 | 0.00 | 0.00 | 0.00 | 0.0000 |
| 2 | 0.00 | 0.00 | 0.00 | 0.0000 |
| 3 | 0.00 | 0.00 | 0.00 | 0.0000 |

**Table 7.19a** Estimated parameters for $p = 3$, 4, 5, 6, and 8

| | *Kxx [m/d]* | *Kyy [m/d]* | *Kxy [m/d]* | *S* |
|---|---|---|---|---|
| Zone | RUN 1, number of complexes, p = 3, simulation efficiency, *eff* = 0.2790E-05 | | | |
| 1 | 0.23108E+02 | 0.27934E+02 | 0.21369E+01 | 0.10707E-02 |
| 2 | 0.30055E+02 | 0.19987E+02 | 0.49419E+01 | 0.30057E-02 |
| 3 | 0.65828E+02 | 0.38419E+02 | 0.31720E+01 | 0.18587E-02 |
| | | | | |
| Zone | RUN 2, number of complexes, $p = 4$, simulation efficiency, *eff* = 0.9477E-06 | | | |
| 1 | 0.35059E+02 | 0.28580E+02 | 0.67120E+00 | 0.16054E-02 |
| 2 | 0.30036E+02 | 0.20057E+02 | 0.36632E+01 | 0.29992E-02 |
| 3 | 0.51796E+02 | 0.36230E+02 | 0.35538E+01 | 0.13559E-02 |
| | | | | |
| Zone | RUN 3, number of complexes, $p = 5$, simulation efficiency, *eff* = 0.7265E-07 | | | |
| 1 | 0.42864E+02 | 0.30561E+02 | 0.24516E+01 | 0.21219E-02 |
| 2 | 0.29998E+02 | 0.19978E+02 | 0.37373E-03 | 0.30012E-02 |
| 3 | 0.49393E+02 | 0.34915E+02 | 0.10186E+01 | 0.89458E-03 |
| | | | | |
| Zone | RUN 4, number of complexes, $p = 6$, simulation efficiency, *eff* = 1.4690E-07 | | | |
| 1 | 0.41278E+02 | 0.30366E+02 | 0.50318E+00 | 0.20723E-02 |
| 2 | 0.29997E+02 | 0.19994E+02 | 0.38413E+00 | 0.29999E-02 |
| 3 | 0.49370E+02 | 0.34745E+02 | 0.16834E+00 | 0.91786E-03 |
| | | | | |
| Zone | RUN 5, number of complexes, $p = 8$, simulation efficiency, *eff* = 0.1672E-08 | | | |
| 1 | 0.39261E+02 | 0.30015E+02 | 0.44779E+00 | 0.19840E-02 |
| 2 | 0.30000E+02 | 0.20002E+02 | 0.11056E+01 | 0.30000E-02 |
| 3 | 0.50458E+02 | 0.35026E+02 | 0.75208E+00 | 0.10000E-02 |

**Table 7.19b** Estimated parameters for $p$ = 10, 12, 15, and 20

| | *Kxx [m/d]* | *Kyy [m/d]* | *Kxy [m/d]* | *S* |
|---|---|---|---|---|
| Zone | RUN 6, number of complexes, $p$ = 10, simulation efficiency, *eff* = 0.2929E-09 | | | |
| 1 | 0.40075E+02 | 0.29993E+02 | 0.15777E+01 | 0.20036E-02 |
| 2 | 0.30000E+02 | 0.20000E+02 | 0.99159E+00 | 0.30000E-02 |
| 3 | 0.49927E+02 | 0.34994E+02 | 0.18454E+01 | 0.99764E-03 |
| | | | | |
| Zone | RUN 7, number of complexes, $p$ = 12, simulation efficiency, *eff* = 0.2930E-09 | | | |
| 1 | 0.40078E+02 | 0.29994E+02 | 0.15801E+01 | 0.20037E-02 |
| 2 | 0.30000E+02 | 0.20000E+02 | 0.99098E+00 | 0.30000E-02 |
| 3 | 0.49926E+02 | 0.34993E+02 | 0.18464E+01 | 0.99755E-03 |
| | | | | |
| Zone | RUN 8, number of complexes, $p$ = 15, simulation efficiency, *eff* = 0.2929E-09 | | | |
| 1 | 0.40075E+02 | 0.29993E+02 | 0.15783E+01 | 0.20035E-02 |
| 2 | 0.30000E+02 | 0.20000E+02 | 0.99206E+00 | 0.30000E-02 |
| 3 | 0.49926E+02 | 0.34994E+02 | 0.18464E+01 | 0.99773E-03 |
| | | | | |
| Zone | RUN 9, number of complexes, $p$ = 20, simulation efficiency, *eff* = 0.2929E-09 | | | |
| 1 | 0.40071E+02 | 0.29993E+02 | 0.15743E+01 | 0.20035E-02 |
| 2 | 0.30000E+02 | 0.20000E+02 | 0.99228E+00 | 0.30000E-02 |
| 3 | 0.49929E+02 | 0.34994E+02 | 0.18421E+01 | 0.99772E-03 |

**Table 7.19c** Estimated parameters for $p$ = 25, 30, 35, and 40

| | *Kxx [m/d]* | *Kyy [m/d]* | *Kxy [m/d]* | *S* |
|---|---|---|---|---|
| Zone | RUN 10, number of complexes, $p$ = 25, simulation efficiency, *eff* = 0.2929E-09 | | | |
| 1 | 0.40075E+02 | 0.29993E+02 | 0.15790E+01 | 0.20035E-02 |
| 2 | 0.30000E+02 | 0.20000E+02 | 0.99172E+00 | 0.30000E-02 |
| 3 | 0.49928E+02 | 0.34994E+02 | 0.18465E+01 | 0.99770E-03 |
| | | | | |
| Zone | RUN 11, number of complexes, $p$ = 30, simulation efficiency, *eff* = 0.2929E-09 | | | |
| 1 | 0.40077E+02 | 0.29993E+02 | 0.15820E+01 | 0.20036E-02 |
| 2 | 0.30000E+02 | 0.20000E+02 | 0.99116E+00 | 0.30000E-02 |
| 3 | 0.49926E+02 | 0.34994E+02 | 0.18487E+01 | 0.99770E-03 |
| | | | | |
| Zone | RUN 12, number of complexes, $p$ = 35, simulation efficiency, *eff* = 0.2929E-09 | | | |
| 1 | 0.40072E+02 | 0.29993E+02 | 0.15738E+01 | 0.20035E-02 |
| 2 | 0.30000E+02 | 0.20000E+02 | 0.99224E+00 | 0.30000E-02 |
| 3 | 0.49928E+02 | 0.34994E+02 | 0.18417E+01 | 0.99769E-03 |
| | | | | |
| Zone | RUN 13, number of complexes, $p$ = 40, simulation efficiency, *eff* = 0.2929E-09 | | | |
| 1 | 0.40074E+02 | 0.29993E+02 | 0.15781E+01 | 0.20035E-02 |
| 2 | 0.30000E+02 | 0.20000E+02 | 0.99205E+00 | 0.30000E-02 |
| 3 | 0.49927E+02 | 0.34994E+02 | 0.18462E+01 | 0.99770E-03 |

**Table 7.20** Summary results of the efficient solutions

| Run Number | Number of complexes | Number of cycles | No of objective function evaluations |
|---|---|---|---|
| 6 | 10 | 181 | 62581 |
| 7 | 12 | 165 | 68386 |
| 8 | 15 | 144 | 75303 |
| 9 | 20 | 135 | 94985 |
| 10 | 25 | 147 | 133466 |
| 11 | 30 | 131 | 137040 |
| 12 | 35 | 147 | 173590 |
| 13 | 40 | 146 | 206189 |

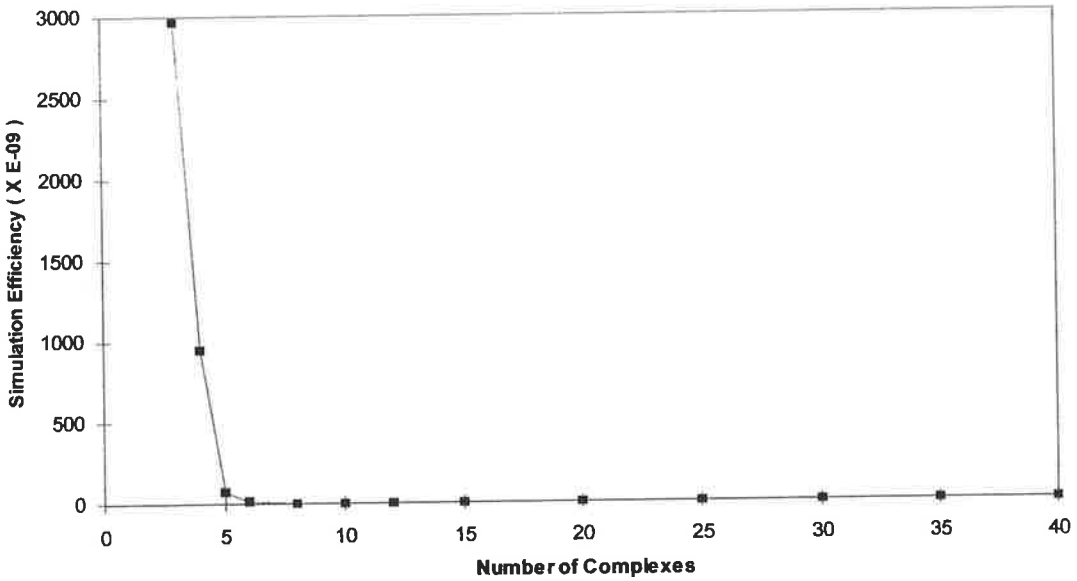



**Figure 7.9** Graphical representation of simulation efficiencies

# 7.6 Summary

This chapter has presented the application of the developed inverse model to field-scale problems. The specific tasks executed include : (1) identification of aquifer formation parameters using two- and three-dimensional flow models; and (2) identification of aquifer formation parameters using two- and three-dimensional solute transport models. Both synthesised and corrupted synthesised data were employed in all analyses. The corrupted

data used in an attempt to emulate data collected from the field in a pumping test experiment. The chapter concluded with a parametric study on the weakness of the SCE methodology by varying the number of complexes over a range of values.

The results obtained in the context of the inverse analysis and with regard to both synthesised and corrupted data were excellent. This does not only indicate the efficiency of the shuffled complex evolution technique but also its potential ability to solve field-scale data. A particular note about the technique is its ability to handle a problem with a parameter dimensionality higher than the number of observation wells. The parametric analyses indicated that the performance of the SCE relies on the proper selection of the number of complexes that controls the entire functioning of the SCE optimisation operation. For more complex problems the parametric study indicated that the SCE fails to find the solution when the number of complexes used in solving the problem is inadequate. However, it is also noted that the use of very large number of complexes result in a solution that is not cost-effective since more computer time is required as a result of the large number of objective function evaluations; but will result in a sensible convergence onto the correct values.

# Chapter 8

# Designation of a Remediation Scheme

## 8.1 Introduction

This chapter deals with the application of the management model developed in the second phase of this research work for the economic design of the number, location, pumping rates, and time of operation of extraction wells in aquifer remediation. As already mentioned, this aspect of the study combines the genetic algorithm (GA) optimisation technique with the finite element method. The entire model comprises (1) a numerical flow model, (2) a numerical solute transport model, and (3) the genetic algorithm optimiser. The numerical model predicts the steady-state hydraulic heads and computes the velocities required by the transport model for the evaluation of the dispersion parameters in the transport governing equation. Given the appropriate parameters, the transport model can be used to determine the extent of contamination of the aquifer before the commencement of the extraction operation. The same transport model also functions as an extraction model when used during the extraction process. The optimiser receives information of concentration levels from the solute transport model during the extraction operation for the optimisation of the number, location, and pumping rates of extraction wells.

It is assumed in the analysis that follows that the parameters used in both the flow and solute transport models are available or could well have been identified by the inverse model of parameter estimation discussed in sections 7.2 and 7.3. Several options exist to reclaim or control a contaminated aquifer. These include in situ bioremediation, slurry walls, pump-and-treat techniques etc. The pump-and-treat technique is relatively inexpensive and accommodates all types of pollutants, whether biodegradable or not. It is therefore assumed that the pump-and-treat strategy is adopted, and that the method of treatment has already been determined.

## 8.2 Problem Statement

A theoretical example is used to illustrate how the management model works. A toxic waste of a specified source strength $100mg/l$ has caused part of an aquifer to become polluted over the past 1000 days. The objective is to determine the extent of the pollution and design a remedial scheme that will reduce the polluted aquifer to acceptable concentration levels most economically.

### 8.2.1 Solution to the Problem

To solve this problem, the hydraulic heads and concentration levels within the aquifer are first predicted using known initial and boundary conditions, and the physical and hydraulic properties of the aquifer. The boundary conditions for both flow and transport models including the spatial discretization of the simulation region are shown in Figure 8.1. The flow model determines the velocities required by the transport model. Heads of $1.5m$ and $0.0m$ are specified at the western and eastern boundaries of the aquifer, respectively. The boundary conditions of the transport model are specified as zero concentration on all

boundaries of the simulation region. The other parameters required for execution of the problem are:

| *Flow Model:* | *value* |
|---|---|
| hydraulic conductivity in x-direction, $k_{xx}$ $[md^{-1}]$ | 20.0 |
| hydraulic conductivity in y-direction, $k_{yy}$ $[md^{-1}]$ | 20.0 |
| aquifer thickness [ $m$] | 20.0 |

| *Transport model :* | *value* |
|---|---|
| longitudinal dispersivity, $\alpha_L$ $[m]$ | 150.0 |
| transverse dispersivity , $\alpha_T$ $[m]$ | 75.0 |
| effective porosity, $\phi$ $[m^3m^{-3}]$ | 0.10 |
| decay constant, $\lambda$ $[d^{-1}]$ | 0.00 |
| coefficient of molecular diffusion $[m^2d^{-1}]$ | 0.00 |
| retardation coefficient, $R$ [-] | 1.00 |

| *GA model* | *value* |
|---|---|
| cost setting up a well, $A$ | \$7000.0 |
| cost of treating a unit volume of water extracted, $B$ | \$5.0 |
| number of individuals per generation | 25 |
| number of generations | 25 |
| probability of crossover, $P_{cross}$ | 0.90 |
| probability of mutation, $P_{mute}$ | 0.01 |

penalty cost for residual pollutant above specified level, $pv$ $1,000,000.00

penalty cost for nodal contaminant levels above the specified level, $p_n$ $100.0

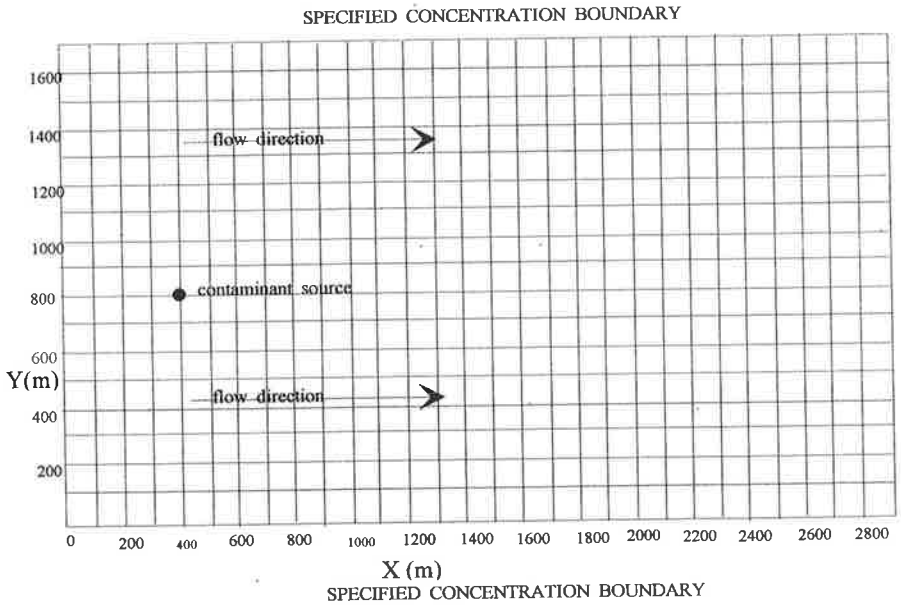



**Figure 8.1** Discretised simulation region showing boundary conditions

The relatively low setting up cost of each well means that the optimisation is effectively to minimise the volume of contaminant water extracted. The concentration levels at the end of 1000 days with a time step of 100 days is shown graphically in Figure 8.2. To design a remedial scheme, a contaminant limit must first be proposed. For the current pollution problem, the constraint measure is to ensure that the concentration levels anywhere within the simulation region will not exceed $5mgl^{-1}$ after the extraction period. The extraction process employs the final concentration levels of the predicted pollution process (Figure 8.2) as its initial input . In a real situation the potential locations of extraction wells would be based on the contaminant distribution of the predicted pollution process (see Figure 8.2) and upon the political and topographical environment. The one- and two-dimensional arrays of potential extraction well locations selected in this exercise are shown in Figures 8.3a

and 8.3b. These locations have been selected on the basis of the concentration distributions shown in Figure 8.2

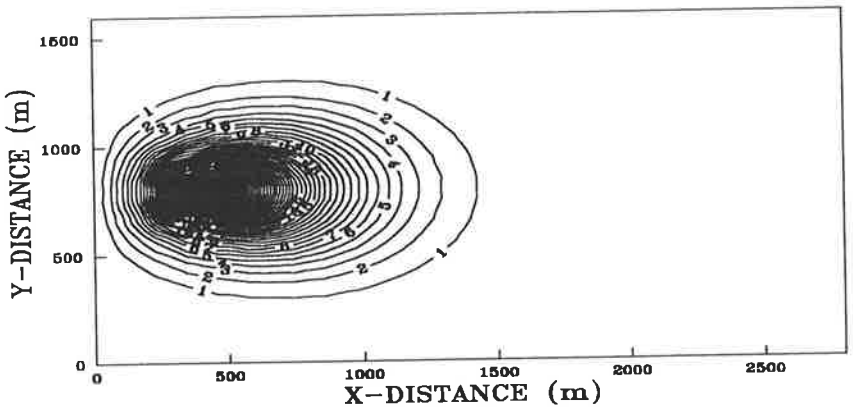
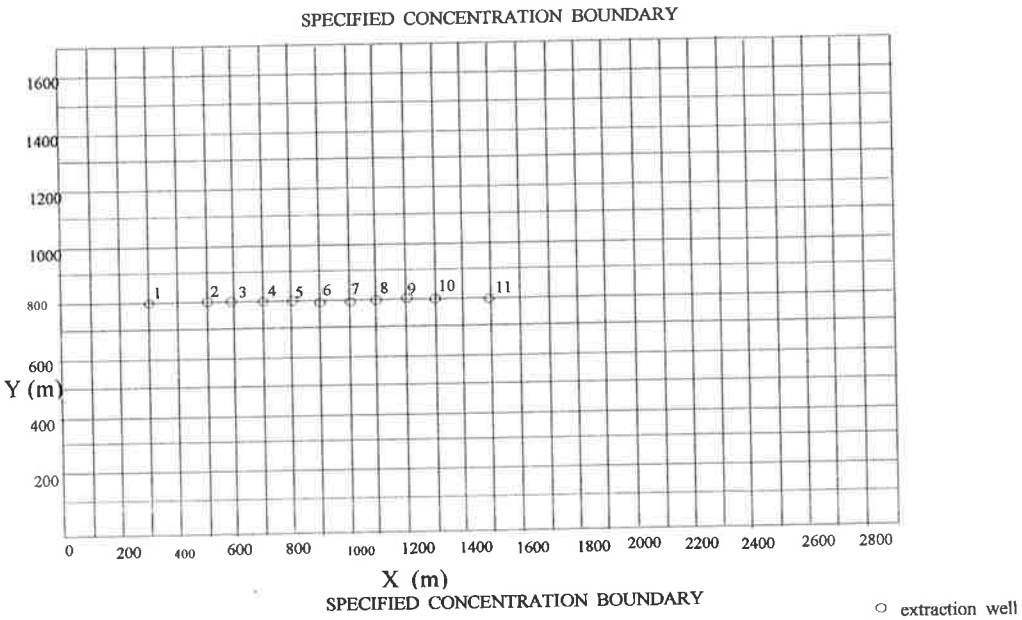



**Figure 8.2** Aquifer concentration distribution before commencement of extraction

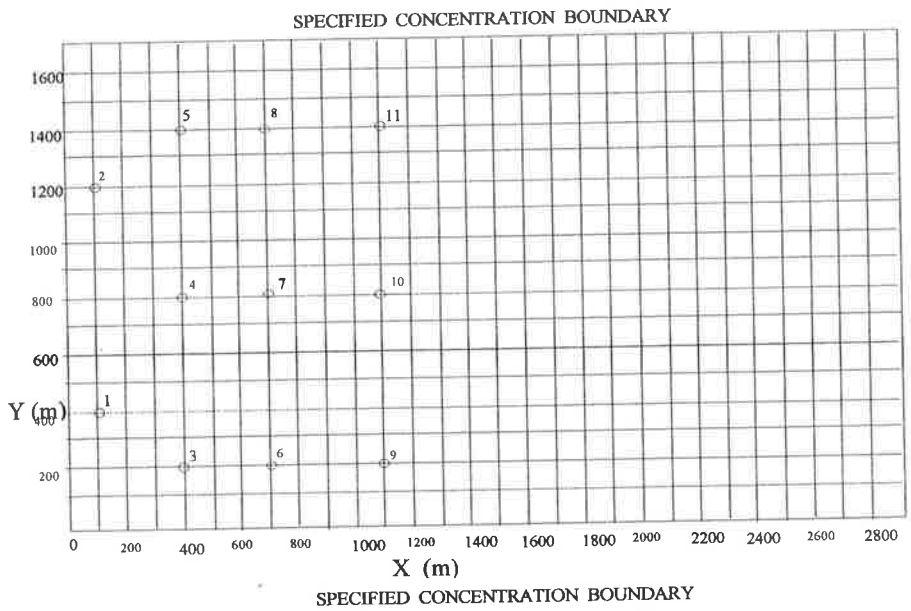
For the one-dimensional well arrangements, a time step of 200 days is set for the numerical model performing the extraction operation and the extraction process is set for a maximum of 20 time steps (4000 days). The pollution must be reduced to below 5 *mg/l* at the end of this extraction period. If this objective is not achieved, the time length set for the extraction operation is increased and the extraction process repeated. In the time-variation scheme, the 20 time steps is partitioned into 6, 7, and 7 (the closest approximation to equal partitioning of integer values of the total number of time steps set for the numerical simulation) for subtime periods $T_1$, $T_2$, and $T_3$, respectively. This implies that for the first six time steps in the numerical model of the time-variation technique, the string allocated to $T_1$ is active in the extraction operation while between time steps 7 and 13 and 14 and 20 strings allocated to $T_2$ and $T_3$ respectively, become active (see Figure 5.5). For the two-dimensional well locations, a maximum of 25 time steps and time step size of 200 days is employed. The sub time intervals for $T_1$, $T_2$, and $T_3$ are respectively 8, 8, and 9 . Using the contaminant constraint condition set by management (ie. the fact the concentration level at each node must not exceed 5 *mg/l* ) the optimal number, location, and pumping rates of extraction wells are

predicted by the GA model. This operation is executed by a repeated exchange of information between the numerical solute transport extraction model and the GA optimiser. This information requires a passage of concentration levels from the numerical model to the GA model; the latter uses the information to identify the optimum number and locations of extraction wells from a population of strings and then passes this information back to the extraction model for the prediction of the nodal concentration levels for the next GA trial. This back and forth passage of information continues until the best optimal solution is found. To determine the effect of allowing pumping rates to vary with time each of the problems was solved with constant pumping rates and the results compared the varying pumping rate solution.

A summary of the solutions generated to remove the contaminant for the one- and two-dimensional potential well arrangements are shown in Tables 8.1 and 8.2 respectively. The concentration distribution for the one-dimensional array at the end of the total extraction period is shown in Figure 8.4 for the nontime varying extraction (constant pumping rates). For the time-varying extraction, the concentration levels at the end the three subtime periods are shown in Figure 8.5. For the two-dimensional array of wells, the concentration distributions are shown in Figure 8.6 for the nontime varying extraction and in Figure 8.7 for the time varying extraction. In these figures, it can be observed that the requirement of reducing the concentration values to below the threshold value of $5mgl^{-1}$ set by management has been achieved. However, the summary results in Tables 8.1 and 8.2 indicate the results obtained from the time-variation technique used in this study is more economical than the nontime variation technique. A graphical representation of the least cost per generation obtained from the GA model shown in Figure 8.8 clearly reveals this fact.




a) one - dimensional




a) two - dimensional

**Figure 8.3** Potential location of extraction wells based on predicted concentration distribution

**Table 8.1** Summary Results of the Extraction Operation with one-dimensional potential extraction well arrangements

| *Constant pumping - one dimensional well arrangements* | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| pumping well numbers | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| pumping rates [ $m^3d^{-1}$] | 25 | 0 | 0 | 75 | 0 | 25 | 0 | 0 | 0 | 0 | 0 |
| remedial cost in $ | 1,521,000.00 | | | | | | | | | | |
| total extraction time [d] | 2400 | | | | | | | | | | |
| *Time variation technique - one dimensional well arrangements* | | | | | | | | | | | |
| pumping well numbers | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| pump rates within $T_1[m^3d^{-1}]$ | 0 | 0 | 0 | 25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| pump rates within $T_2[m^3d^{-1}]$ | 0 | 0 | 0 | 0 | 0 | 25 | 0 | 0 | 0 | 0 | 0 |
| pump rates within $T_3[m^3d^{-1}]$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 25 | 0 | 0 |
| cost in $ | 1,104,700.00 | | | | | | | | | | |
| total extraction time [*d*] | 2800 | | | | | | | | | | |

**Table 8.2** Summary Results of the Extraction Operation with two-dimensional potential extraction well arrangements

| *Constant pumping - two dimensional well arrangements* | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| pumping well numbers | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| pumping rates [ $m^3d^{-1}$] | 0 | 0 | 0 | 50 | 0 | 0 | 25 | 25 | 0 | 25 | 0 |
| remedial cost in $ | 1,828,000.00 | | | | | | | | | | |
| total extraction time [*d*] | 2400 | | | | | | | | | | |
| *Time variation technique - two dimensional well arrangements* | | | | | | | | | | | |
| pumping well numbers | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| pump rates within $T_1[m^3d^{-1}]$ | 0 | 0 | 0 | 25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| pump rates within $T_2[m^3d^{-1}]$ | 0 | 0 | 0 | 0 | 25 | 0 | 0 | 0 | 0 | 0 | 0 |
| pump rates within $T_3[m^3d^{-1}]$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 25 | 25 | 25 |
| cost in $ | 1,535,000.00 | | | | | | | | | | |
| total extraction time [*d*] | 2200 | | | | | | | | | | |

It can be seen that in both one- and two-dimensional arrangements, the time variation technique yielded a better results. From cost considerations, the one-dimensional arrangements of the extraction wells appears to be the better of the two alternatives. It is recognised, however, that there can be no guarantee that a GA solution is the global optimum but that the generated solution is of reasonable efficiency which may be used as a starting point for further investigation. The fact that the time-variation scheme generates a more efficient solution than the nontime variation scheme greatly assists in achieving an eventual

solution of high efficiency. The improvement in cost savings results from a reduced redundancy effect of the extraction wells as contaminant plumes move along during the numerical simulation process.

The study has demonstrated that a better remedial design for pollutant extraction can be achieved if the pumping sequences of active wells are permitted to vary with time. Dividing the extraction period into three sub periods produced a 27% and 16% savings in costs for the one- and two-dimensional arrangements of extraction wells, respectively, over their respective fixed pumping regimes. However, irrespective of any of the conclusions drawn, it is the judgement of the engineer/hydrologist in selecting possible well positions (using the predicted concentration contour map derived from the analysis, ie., Figure 8.2), for the GA to optimise, that is critical if any hope of a realistic solution is to be achieved with an acceptable amount of computer effort.

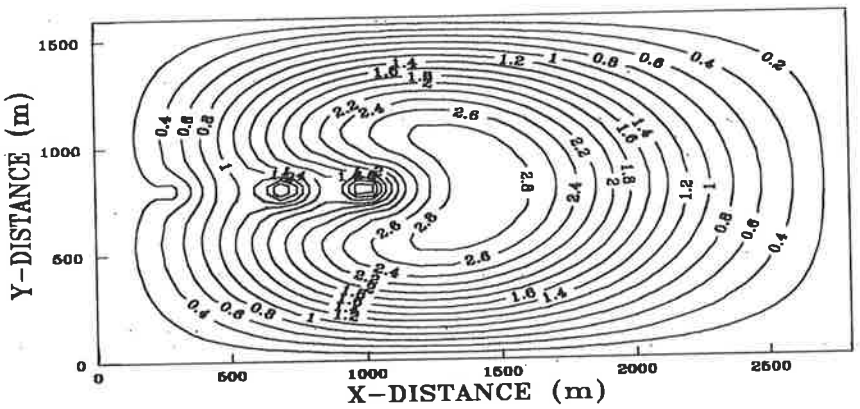



**Figure 8.4** Concentration distribution at the end of extraction period for nontime-variation with well arrangements in one-dimension.

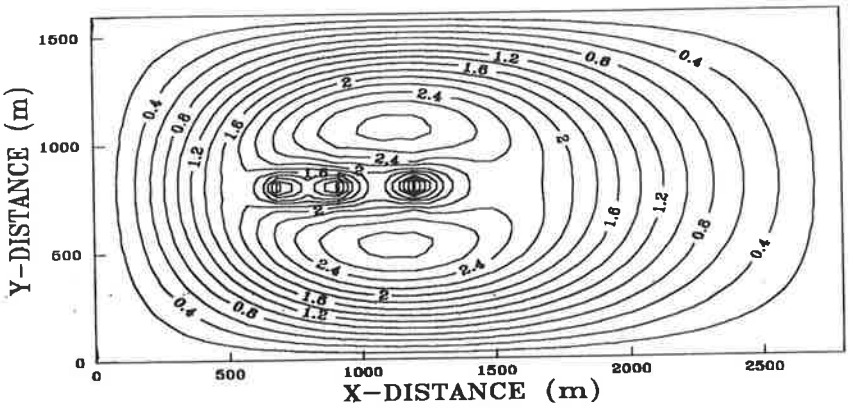



**Figure 8.5** Concentration distribution at the end of time interval T3 of the time-variation scheme with well arrangements in one-dimension.

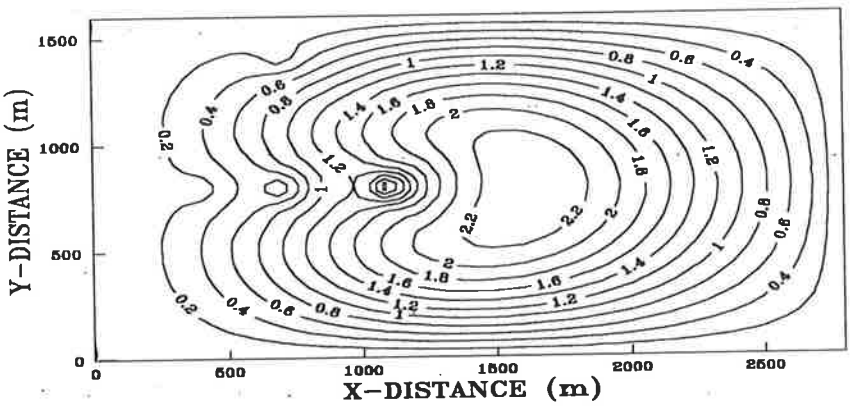



**Figure 8.6** Concentration distribution at the end of extraction period for non-time variation scheme with well arrangements in two-dimension.

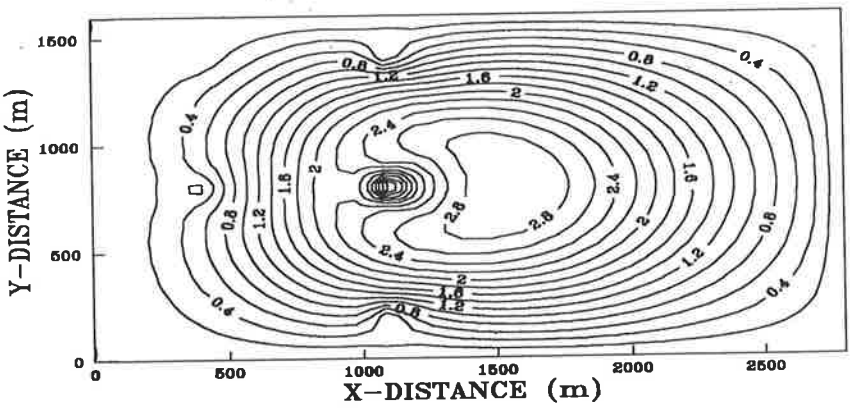



**Figure 8.7** Concentration distribution at the end of time interval T3 of the time-variation scheme with well arrangements in two-dimensions.

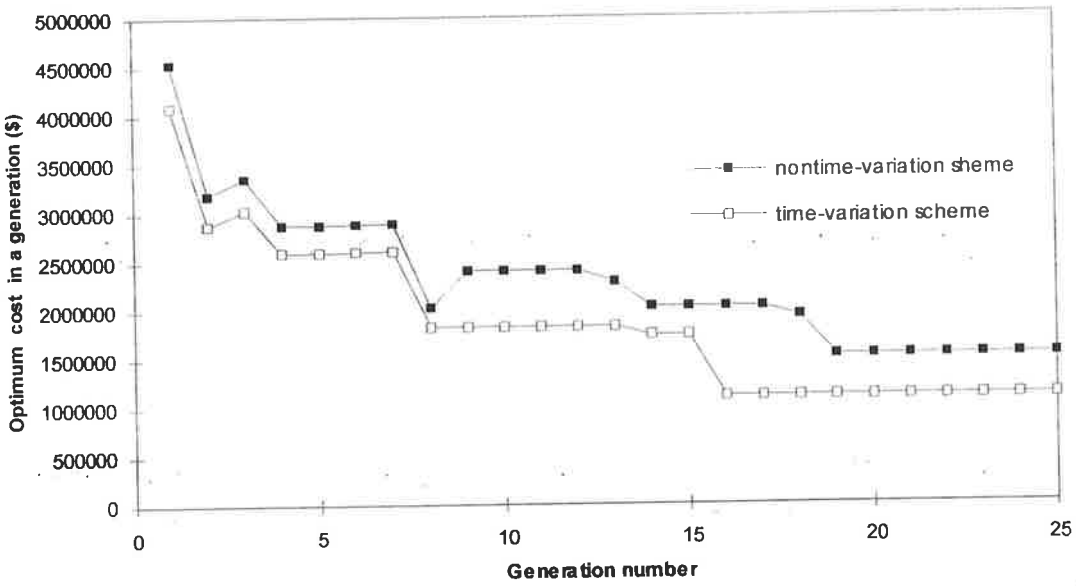



**Figure 8.8a** Optimum cost in a generation for one-dimensional well arrangements

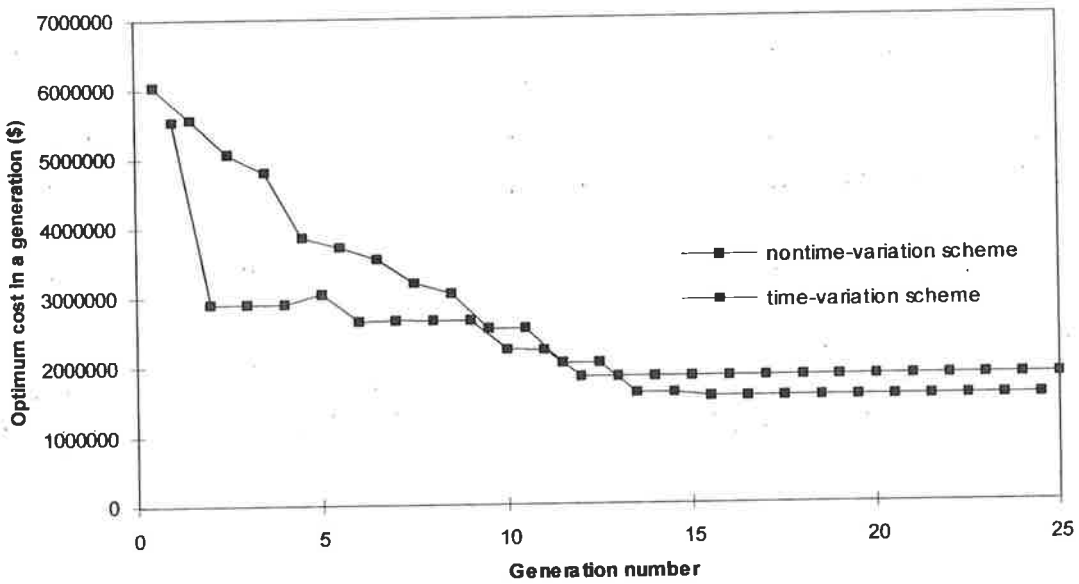



**Figure 8.8b** Optimum cost in a generation for two-dimensional well arrangements

# 8.3 Summary

This chapter has demonstrated the application of the management model to the extraction of contaminants in a polluted aquifer. Two techniques namely (1) nontime variation and (2) the time variation in the context of both one- and two-dimensional potential arrangements of the extraction wells have been used to demonstrate how the management model works . More importantly, the demonstration has shown that a better remedial design for pollutant extraction can be achieved if the active wells are permitted to vary with time by dividing the total extraction period into a number of sub time periods. The analyses performed in the context of one- and two-dimensional potential arrangements of the extraction wells, have both indicated that the time variation technique produces a more economic cost than the nontime variation technique. However, irrespective of any of these conclusions drawn, it is the responsibility of the engineer/hydrologist in selecting possible potential well positions (using the predicted concentration contour map derived from the analysis) for the GA to optimise, that is critical, if any hope of a realistic solution is to be achieved.

# Chapter 9

# Research Conclusions, Recommendations, and Contribution

## 9.1 Conclusion

The research was initiated with the objective of improving the state of the science in the inverse problem of parameter identification and contaminant remediation design schemes through the use of modern evolutionary techniques. The specific task that were accomplished are: (1) the formulation and designation of a model for the inverse problem of parameter identification using the shuffled complex evolutionary technique for two- and three-dimensional flow and solute transport models; (2) the formulation and designation of a management-oriented model using another evolutionary technique called genetic algorithm for remediation design schemes in contaminant extraction processes, and (3) evaluation and application of these models to field and hypothetical data. Several important conclusions can be drawn from the results of this research study.

- The present inverse model was used to test a variety of problems from the analytical and the numerical point of view using field, synthesised, and corrupted synthesised data. The results of all the analyses indicated that the shuffled complex evolutionary technique is robust, efficient, and effective; and works not only for the calibration of conceptual rainfall and runoff models but also for inverse problem of groundwater

modelling as well. The technique can thus serve as a very useful alternative to the traditional gradient-based techniques that has been used for the inverse problem of parameter identification in the past three decades.

- Some major problems that have still not been resolved in the use of the gradient-based methods for the inverse problem of parameter identification are the effects of singularity and ill-conditioning (near singularity) of the sensitivity matrix. These problems usually happen when the inverse of the sensitivity matrix ceases to exist (ie. when its determinant becomes zero or very close to zero) or when the problem under consideration is highly nonlinear. The shuffled complex evolution performs its search for the optimal solution through the use of random elements. It requires no computation of gradients (or sensitivity matrix). Therefore in the context parameter sensitivity and interaction and problem nonlinearity, the shuffled complex evolution may be considered to be superior to the traditional gradient-based methods.

- Another major problem with the gradient-based method of parameter identification is the instability of the parameters under estimation in the course of the optimisation process. It has been documented that such problems are caused by a smaller number of observation nodes or wells as compared to the parameter dimensionality of the problem. In fact, in all but analysis 1 and analysis 5 of the problems solved in chapter seven, the number of observation wells or nodes have always been smaller than the parameter dimensionality of the problem under consideration. Therefore, in the event of a situation where the available number of observation wells or nodes are smaller than the number of parameters to be estimated, the shuffled complex evolutionary technique may be a suitable candidate for the problem.

- One area in the inverse problem of parameter identification that has received relatively little attention is the estimation of solute transport parameters in the numerical modelling context. This may be attributed to the potential problems expected in the use of the solute transport model - which even in its forward mode only, posses numerical problems in some analysis. The versatility, flexibility, robustness, and efficiency of the shuffled complex evolutionary technique used in this research study has permitted the estimation of solute transport parameters not only in the two-dimensional context but in three-dimensions as well.

- It was however, detected that the shuffled complex evolutionary technique fails when the population of points initialised in the parameter search space are inadequate. The number of population of points initialised in the search space is controlled by a parameter which determines the number of complexes or communities $p$, required to solve a given problem. If $p$ is too small, a sparsely populated parameter search spaced is initialised, leaving the optimiser with an insufficient number of points to optimise from. On the other hand, if $p$ is selected to be too large, a densely populated parameter search space is initialised, leaving the optimiser with too many points (and hence too many objective function evaluations) to optimise from. Although, the latter case will always converge to the right solution, it does so with excessive amount of computational time and effort; resulting in a solution that is not cost-effective. Experience in this research has however shown that, with known number of parameters under estimation $n$, a convergence and cost-effective solution can be achieved if an optimal number of complexes $p_{opt}$, is selected such that: $n-2 \leq p_{opt} \leq n+2$.

- In the context of the management model, results have indicated that the genetic algorithm approach is suitable for extraction operations. Because of the structure of

its design, the optimisation of more parameters (such as location, pumping rate, number of extraction wells, and above all the cost of the entire scheme) could be accommodated within a single run. The two extraction methods adopted - time variation and nontime variation technique - were all capable of yielding the desired optimum solution. However, the time variation technique yielded a better economic results. This better performance of the time variation technique is attributed to the fact that the effect of well redundancy as contaminant plumes move along could be effectively nullified by partitioning the entire simulation period into smaller subtime periods and allocating a string (or decision variable) to each. Although solutions obtained from each of these techniques can not be guaranteed to be the global optimum, they can serve as initial starting points for further investigations or can be implemented without further investigation.

- Because natural processes cannot be accurately modelled by physical or mathematical models, it is appropriate to mention that the judgment of the analyst in selecting appropriate potential well locations for the management model to use in the optimisation is a very crucial factor in the use of this model. This burden has been reduced in the present management model by the fact that the contaminant distribution of the area under consideration can first be predicted - given a knowledge of the physical, hydraulic, initial, and boundary conditions - before commencement of the extraction process. The contours of the concentration distribution - which serve as input to the extraction operation - can then be used as a guide for the analyst in the selection of the appropriate potential well locations.

## 9.2 Recommendations

The following improvement and extensions to the present work are recommended in future research:

- In the context of the inverse problem of parameter identification, the only field data used in parameter estimation was applied to the Theis analytical model. This was due to the lack of sufficient information (eg boundary and initial conditions, and the areas extent of the aquifer) regarding the area in which the field pumping test data was collected. Although corrupted synthetic data have been used in all parameter estimation applications in this work to emulate field pumping test data, the need to apply the model to real field pumping test data is required to boost up the confidence in the use of shuffled complex evolution for future parameter identification programs in the context of numerical groundwater modelling.

- One major problem with the application of the shuffled complex evolutionary technique in parameter estimation analysis is the length of time required to complete more difficult and complicated problems. For very simple homogeneous problems, though, simulation can be completed within a matter of seconds. The large amount of time required for complicated problems is due to the large number of objective function evaluations that are performed in the course of the optimisation process. In this regard, it is recommended that the shuffled complex technique of parameter estimation in numerical models be extended onto parallel computers, where the large number of function evaluations could be shared among the available multiprocessors. This will produce a dramatic reduction of computational time.

- The finite element method used in this research work is a domain approach, wherein the region to be modelled is divided into a large number of nodes, resulting in a large number of equations that require a great amount of computational effort, time, storage, data preparation and handling. The boundary element method of numerical analysis is based on integral equation formulation of boundary value problems and requires discretization of only the boundary and not the interior of the region under consideration. This lessens the computational burden and increases computational efficiency by virtue of the fact that the order of geometrical dimensionality reduces by one. Furthermore, the boundary element technique allows the analyst to simulate only areas of interest in the simulation region - making it more suitable for the solution of the inverse problem where only a few predicted nodes of the observation wells are required for the inverse analysis. Therefore in the absence of parallel computers it is recommended that the shuffled complex evolution technique of solving the inverse problem of parameter identification be interfaced with the boundary element method for savings of computational time in future research.

- It turned out that the time variation technique used as an alternative to the nontime variation technique yielded a better results by partitioning the entire number of simulation times to three subtime intervals. This number of time partitioning were used for the sake of computational storage. Future research studies should consider the use of more subtime intervals or the use of the more advanced messy genetic algorithm whose method of 'cut' and 'splice' method of generating offsprings (or decision variables) can be used as an alternative method that can be used to vary the pumping regimes of the chromosomes or strings instead of the time variation method used in this research work.

- Like the numerical part of the inverse model, only a theoretical example has been used to demonstrate the performance of the management model. It is recommended that future continuation of this work should consider applying the model to practical field work. It is only through this that the performance of the management model can be assessed.

## 9.3 Research Contribution of this Project

For the first time in the inverse problem of parameter identification in groundwater modelling an entirely new evolutionary technique that promises to be very robust, effective, and efficient has been used. The shuffled complex evolutionary technique was developed by *Duan et al.* [1992,1993] at the University of Arizona and used exclusively for the calibration of complex conceptual rainfall-runoff in surface modelling. Realising that the method has been used by several researchers with considerable success in the calibration of surface runoff models, it was decided to modify and extend the methodology into groundwater modelling for the inverse problem of parameter identification. Unexpectedly, the methodology does not only work in groundwater modelling but works very well.

Special credit goes to its ability to handle three-dimensional models which in the past have been given relatively little attention. This is not because they are too difficult to handle but rather the problems associated with the various forms of the traditional gradient-based methods that are used to solve inverse problem. It is hoped that further research in the area of the shuffled complex evolutionary technique with regard to the inverse problem of parameter identification could result in a more efficient optimisation tool that could help handle the solution difficulties encountered in the use of the gradient-based techniques.

It was identified in the literature survey that the major problems associated with the traditional gradient-based method of groundwater management was the inability of the models to handle more constraints owing to the resultant formulation of large response matrices. The current genetic algorithm technique used in the optimisation model does not handle the optimisation problem with matrix computation. All its optimisation processes are stochastical (the use of random elements). The time variation method was a technique used in this work after realising that the movement of contaminant plumes as simulation time progress could render some of the operating extraction wells redundant if their locations and rates of extraction are permitted to vary with time. The sample simulation presented in chapter eight has confirmed (in both one- and two-dimensional potential arrangement of extraction wells) that the time variation technique was more effective than the nontime variation technique. The revelation here may serve as a useful gateway as to the need to vary the status of the decision variables represented on the strings or chromosomes in dynamic simulation modelling with genetic algorithm for a better optimum results in future research studies.

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# Appendices

Appendix 1a Synthesized data for analysis 1

| Synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 21 | node 53 | node 93 | node 107 |
| 1.00 | 0.11831 | 0.21115 | 0.30613 | 0.08494 |
| 2.00 | 0.13600 | 0.23621 | 0.34113 | 0.09623 |
| 3.00 | 0.13777 | 0.23857 | 0.34402 | 0.09728 |
| 4.00 | 0.13799 | 0.23911 | 0.34456 | 0.09740 |
| 5.00 | 0.13812 | 0.23957 | 0.34497 | 0.09747 |
| 6.00 | 0.13823 | 0.23996 | 0.34531 | 0.09752 |
| 7.00 | 0.13831 | 0.24030 | 0.34558 | 0.09756 |
| 8.00 | 0.13838 | 0.24059 | 0.34581 | 0.09760 |
| 9.00 | 0.13845 | 0.24084 | 0.34601 | 0.09763 |
| 10.00 | 0.13850 | 0.24106 | 0.34617 | 0.09766 |

Appendix 1b Corrupted data for analysis 1

| Synthesized corrupted drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 21 | node 53 | node 93 | node 107 |
| 1.00 | 0.11810 | 0.21305 | 0.30493 | 0.08683 |
| 2.00 | 0.13597 | 0.23518 | 0.34208 | 0.09307 |
| 3.00 | 0.13769 | 0.23956 | 0.34321 | 0.09410 |
| 4.00 | 0.13798 | 0.23996 | 0.34400 | 0.09537 |
| 5.00 | 0.13812 | 0.24035 | 0.34525 | 0.09623 |
| 6.00 | 0.13807 | 0.23980 | 0.34575 | 0.09827 |
| 7.00 | 0.13827 | 0.24087 | 0.34641 | 0.09835 |
| 8.00 | 0.13832 | 0.24099 | 0.34768 | 0.09851 |
| 9.00 | 0.13836 | 0.24180 | 0.34779 | 0.09554 |
| 10.00 | 0.13832 | 0.24295 | 0.34806 | 0.09843 |

Appendix 2a Synthesized data for analysis 2

| Synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 50 | node 60 | node 62 | node 72 |
| 1.00 | 1.19621 | 0.79348 | 0.83391 | 1.11820 |
| 2.00 | 1.51050 | 1.08494 | 1.14077 | 1.54705 |
| 3.00 | 1.60665 | 1.17842 | 1.24312 | 1.69004 |
| 4.00 | 1.64066 | 1.21206 | 1.28139 | 1.74215 |
| 5.00 | 1.65319 | 1.22456 | 1.29598 | 1.76147 |
| 6.00 | 1.65848 | 1.23004 | 1.30242 | 1.76933 |
| 7.00 | 1.66005 | 1.23164 | 1.30432 | 1.77162 |
| 8.00 | 1.66131 | 1.23302 | 1.30594 | 1.77342 |
| 9.00 | 1.66238 | 1.23423 | 1.30734 | 1.77489 |
| 10.00 | 1.66330 | 1.23530 | 1.30857 | 1.77612 |

Appendix 2b Corrupted data for analysis 2

| Corrupted synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 50 | node 60 | node 62 | node 72 |
| 1.00 | 1.21635 | 0.75297 | 0.84405 | 1.15870 |
| 2.00 | 1.55059 | 1.09461 | 1.10081 | 1.49634 |
| 3.00 | 1.61754 | 1.16776 | 1.21328 | 1.67025 |
| 4.00 | 1.63209 | 1.20201 | 1.29151 | 1.75211 |
| 5.00 | 1.64329 | 1.23519 | 1.31556 | 1.76167 |
| 6.00 | 1.64819 | 1.24048 | 1.32352 | 1.76824 |
| 7.00 | 1.66556 | 1.24186 | 1.35430 | 1.76995 |
| 8.00 | 1.66878 | 1.24525 | 1.37543 | 1.77552 |
| 9.00 | 1.67037 | 1.24714 | 1.38776 | 1.77822 |
| 10.00 | 1.66743 | 1.24965 | 1.41896 | 1.77994 |

Appendix 3a Synthesized data for analysis 3

| Synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 50 | node 60 | node 62 | node 72 |
| 1.00 | 0.40659 | 0.17182 | 0.17187 | 0.40658 |
| 2.00 | 0.81984 | 0.49258 | 0.49351 | 0.81988 |
| 3.00 | 1.08372 | 0.71045 | 0.71367 | 1.08391 |
| 4.00 | 1.26129 | 0.86239 | 0.86924 | 1.26174 |
| 5.00 | 1.38792 | 0.97202 | 0.98331 | 1.38865 |
| 6.00 | 1.48140 | 1.05313 | 1.06914 | 1.48239 |
| 7.00 | 1.55174 | 1.11405 | 1.13462 | 1.55292 |
| 8.00 | 1.60517 | 1.16016 | 1.18487 | 1.60649 |
| 9.00 | 1.64591 | 1.19516 | 1.22344 | 1.64730 |
| 10.00 | 1.67777 | 1.22306 | 1.25448 | 1.67919 |

Appendix 3b Corrupted data for analysis 3

| Corrupted synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 50 | node 60 | node 62 | node 72 |
| 1.00 | 0.43673 | 0.16131 | 0.16201 | 0.41707 |
| 2.00 | 0.83992 | 0.48222 | 0.51355 | 0.83917 |
| 3.00 | 1.06459 | 0.72979 | 0.70382 | 1.07412 |
| 4.00 | 1.25271 | 0.87235 | 0.85935 | 1.25170 |
| 5.00 | 1.39802 | 0.98265 | 0.97289 | 1.36885 |
| 6.00 | 1.46111 | 1.03357 | 1.08024 | 1.49229 |
| 7.00 | 1.57225 | 1.12427 | 1.12460 | 1.54225 |
| 8.00 | 1.59564 | 1.16939 | 1.19436 | 1.59659 |
| 9.00 | 1.65590 | 1.18057 | 1.23385 | 1.65762 |
| 10.00 | 1.69790 | 1.24440 | 1.26488 | 1.69902 |

Appendix 4a Synthesized data for analysis 4

| Synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 200 | node 240 | node 248 | node 288 |
| 1.00 | 1.91152 | 0.76258 | 0.75156 | 1.85971 |
| 2.00 | 2.98138 | 1.73702 | 1.72674 | 2.93661 |
| 3.00 | 3.48803 | 2.23882 | 2.23405 | 3.47996 |
| 4.00 | 3.77473 | 2.53366 | 2.53557 | 3.80642 |
| 5.00 | 3.95026 | 2.71840 | 2.72695 | 4.01658 |
| 6.00 | 4.06319 | 2.83882 | 2.85288 | 4.15602 |
| 7.00 | 4.13691 | 2.91801 | 2.93667 | 4.24934 |
| 8.00 | 4.18632 | 2.97123 | 2.99326 | 4.31244 |
| 9.00 | 4.22044 | 3.00975 | 3.03222 | 4.35579 |
| 10.00 | 4.24198 | 3.03113 | 3.05753 | 4.38417 |

Appendix 4b Corrupted data for analysis 4

| Corrupted synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 200 | node 240 | node 248 | node 288 |
| 1.00 | 1.85167 | 0.75310 | 0.65170 | 1.86721 |
| 2.00 | 2.99147 | 1.83736 | 1.74677 | 2.91735 |
| 3.00 | 3.58895 | 2.13949 | 2.13421 | 3.45988 |
| 4.00 | 3.76622 | 2.55361 | 2.33568 | 3.82637 |
| 5.00 | 3.96036 | 2.77905 | 2.70738 | 4.00679 |
| 6.00 | 4.05349 | 2.81927 | 2.75401 | 4.12593 |
| 7.00 | 4.14745 | 2.95842 | 2.95665 | 4.23004 |
| 8.00 | 4.17682 | 2.96203 | 2.89378 | 4.33255 |
| 9.00 | 4.20043 | 3.01785 | 3.07265 | 4.33614 |
| 10.00 | 4.25211 | 3.02252 | 3.08794 | 4.37399 |

Appendix 5a Synthesized data for analysis 5

| Synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 50 | node 60 | node 62 | node 72 |
| 10.00 | 20.63188 | 12.71832 | 7.88860 | 6.93689 |
| 20.00 | 28.00738 | 19.95068 | 14.36957 | 13.36723 |
| 30.00 | 30.50647 | 23.13350 | 17.90091 | 17.17352 |
| 40.00 | 31.41902 | 24.47695 | 19.56609 | 19.07175 |
| 50.00 | 31.77680 | 25.04752 | 20.30989 | 19.95297 |
| 60.00 | 31.92421 | 25.29346 | 20.63660 | 20.35069 |
| 70.00 | 31.98698 | 25.40108 | 20.78012 | 20.52869 |
| 80.00 | 32.01427 | 25.44861 | 20.84335 | 20.60834 |
| 90.00 | 32.02630 | 25.46977 | 20.87138 | 20.64406 |
| 100.00 | 32.03167 | 25.48935 | 20.90401 | 20.66016 |

Appendix 5b Corrupted data for analysis 5

| Corrupted synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 50 | node 60 | node 62 | node 72 |
| 10.00 | 20.76795 | 12.60842 | 7.69075 | 6.90090 |
| 20.00 | 28.10103 | 19.84586 | 14.46327 | 13.48489 |
| 30.00 | 30.58704 | 23.23423 | 17.89359 | 17.28906 |
| 40.00 | 31.41762 | 24.58604 | 19.59113 | 19.03686 |
| 50.00 | 31.77599 | 25.09083 | 20.19001 | 19.96156 |
| 60.00 | 31.96417 | 25.35668 | 20.69858 | 20.34100 |
| 70.00 | 31.97650 | 25.41423 | 20.80785 | 20.53431 |
| 80.00 | 31.98840 | 25.45500 | 20.83474 | 20.56421 |
| 90.00 | 32.00360 | 25.46678 | 20.88798 | 20.61978 |
| 100.00 | 32.24773 | 25.48428 | 20.89621 | 20.68654 |

Appendix 6a Synthesized data for analysis 6

| Synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 50 | node 60 | node 62 | node 72 |
| 5.00 | 11.64825 | 6.94897 | 3.94806 | 3.34257 |
| 10.00 | 17.13160 | 11.79601 | 8.08330 | 7.18624 |
| 15.00 | 19.66686 | 14.56718 | 11.03398 | 10.11704 |
| 20.00 | 20.96420 | 16.15485 | 12.91674 | 12.07092 |
| 25.00 | 21.68560 | 17.09066 | 14.07845 | 13.31660 |
| 30.00 | 22.11019 | 17.65954 | 14.79747 | 14.10533 |
| 35.00 | 22.37223 | 18.01837 | 15.25461 | 14.61235 |
| 40.00 | 22.53803 | 18.24842 | 15.54844 | 14.94160 |
| 45.00 | 22.64463 | 18.39761 | 15.73913 | 15.15696 |
| 50.00 | 22.71630 | 18.49908 | 15.86930 | 15.30273 |

Appendix 6b Corrupted data for analysis 6

| Corrupted synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 50 | node 60 | node 62 | node 72 |
| 5.00 | 11.75833 | 6.84622 | 4.05110 | 3.14112 |
| 10.00 | 17.02965 | 11.69459 | 8.18153 | 7.19999 |
| 15.00 | 19.56059 | 14.66810 | 11.00864 | 10.10156 |
| 20.00 | 20.76373 | 16.26445 | 13.01780 | 12.04937 |
| 25.00 | 21.68632 | 17.10544 | 14.00656 | 13.30947 |
| 30.00 | 22.12402 | 17.64113 | 14.70894 | 14.11930 |
| 35.00 | 22.32857 | 18.00326 | 15.26479 | 14.62403 |
| 40.00 | 22.49644 | 18.25654 | 15.65642 | 14.83947 |
| 45.00 | 22.61661 | 18.38972 | 15.70893 | 15.12472 |
| 50.00 | 22.78263 | 18.51106 | 15.89754 | 15.31621 |

Appendix 7a Synthesized data for analysis 7

| Synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 48 | node 56 | node 88 | node 96 |
| 20.00 | 26.83890 | 1.24140 | 0.65688 | 46.84318 |
| 40.00 | 28.13749 | 3.75310 | 1.16032 | 55.56329 |
| 60.00 | 28.31579 | 5.25457 | 1.36259 | 58.35655 |
| 80.00 | 28.37079 | 6.01221 | 1.43500 | 59.36422 |
| 100.00 | 28.39262 | 6.37823 | 1.46144 | 59.74749 |
| 120.00 | 28.40184 | 6.54952 | 1.47148 | 59.89908 |
| 140.00 | 28.40618 | 6.62715 | 1.47569 | 59.96452 |
| 160.00 | 28.40819 | 6.66246 | 1.47751 | 59.99280 |
| 180.00 | 28.40918 | 6.67902 | 1.47839 | 60.00655 |
| 200.00 | 28.40962 | 6.68611 | 1.49877 | 60.01249 |

Appendix 7b Corrupted data for analysis 7

| Corrupted synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 50 | node 60 | node 62 | node 72 |
| 20.00 | 26.64212 | 1.13990 | 0.65739 | 46.72297 |
| 40.00 | 28.11430 | 3.69964 | 1.16107 | 55.68999 |
| 60.00 | 28.30977 | 5.36454 | 1.36193 | 58.59994 |
| 80.00 | 28.37116 | 6.08579 | 1.43405 | 59.25661 |
| 100.00 | 28.39186 | 6.39375 | 1.46073 | 59.79527 |
| 120.00 | 28.40261 | 6.59382 | 1.47292 | 59.88840 |
| 140.00 | 28.40453 | 6.60917 | 1.47668 | 59.97655 |
| 160.00 | 28.40714 | 6.62968 | 1.47727 | 59.99522 |
| 180.00 | 28.41011 | 6.65098 | 1.47864 | 50.00580 |
| 200.00 | 28.42004 | 6.70321 | 1.47864 | 60.12534 |

Appendix 8a Synthesized data for analysis 8

| Synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 96 | node 104 | node 152 | node 160 |
| 20.00 | 36.11600 | 4.41404 | 0.09457 | 27.94942 |
| 40.00 | 39.49862 | 7.31205 | 1.94628 | 34.85157 |
| 60.00 | 40.26950 | 8.99200 | 3.65153 | 38.43368 |
| 80.00 | 40.59460 | 9.98476 | 4.84773 | 40.59979 |
| 100.00 | 40.77600 | 10.59684 | 5.62922 | 41.97280 |
| 120.00 | 40.88826 | 10.98886 | 6.13209 | 42.86011 |
| 140.00 | 40.96082 | 11.24702 | 6.45598 | 43.44103 |
| 160.00 | 41.00879 | 11.42015 | 6.66615 | 43.82492 |
| 180.00 | 41.04091 | 11.53760 | 6.80371 | 44.08043 |
| 200.00 | 41.06258 | 11.61775 | 6.89444 | 44.25128 |

Appendix 8b Corrupted data for analysis 8

| Corrupted synthesized drawdown data [m] | | | | |
|---|---|---|---|---|
| Time [days] | node 96 | node 104 | node 152 | node 160 |
| 20.00 | 36.23162 | 4.51317 | 0.08660 | 27.93739 |
| 40.00 | 39.53638 | 7.42161 | 1.83207 | 34.86308 |
| 60.00 | 40.17909 | 9.09000 | 3.75047 | 38.33368 |
| 80.00 | 40.58815 | 10.02773 | 3.94622 | 40.69979 |
| 100.00 | 40.88074 | 10.62142 | 5.61922 | 41.89309 |
| 120.00 | 40.90105 | 10.99247 | 6.23477 | 42.98133 |
| 140.00 | 40.95747 | 11.18449 | 6.48813 | 43.46088 |
| 160.00 | 41.01837 | 11.39863 | 6.65786 | 43.79741 |
| 180.00 | 41.03564 | 11.52669 | 6.79699 | 44.00281 |
| 200.00 | 41.17234 | 11.58524 | 6.87679 | 44.35077 |