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Sensitivity analysis of groundwater flow.

Licentiate thesis

Yung-Bing Bao

Royal Institute of Technology, Department of Land and Water Resources, Stockholm, Sweden

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SWEDISH NUCLEAR FUEL AND WASTE MANAGEMENT CO

BOX 5864 S-102 48 STOCKHOLM

TEL 08-665 28 00 TELEX 13108 SKB S
TELEFAX 08-661 57 19

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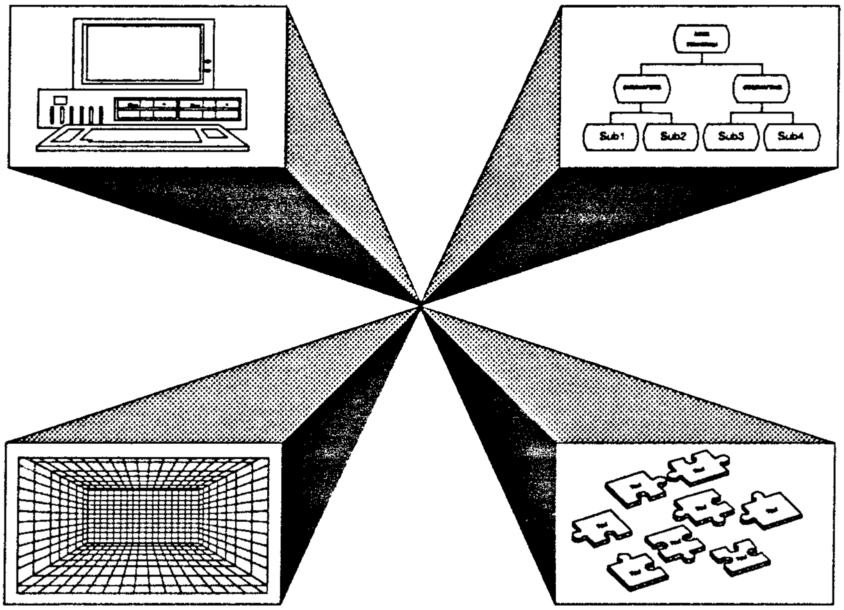

YUNG-BING BAO

Royal Institute of Technology
Department of Land and Water Resources
Stockholm Sweden

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ABSTRACT

Sensitivity is usually defined as a derivative of a specific performance measure with respect to the system parameters. Sensitivity analysis is an effective tool for analysing the responses of some selected performance measure of a groundwater flow problem to perturbations of the parameters. It is used to study the behaviour of flow systems and to assess the importance of the various governing flow parameters.

A sensitivity analysis of general linear and nonlinear simulation equation sets is developed in this study in order to facilitate the application of the sensitivity analysis to groundwater flow problems. Two methods are considered for the sensitivity calculation: the "direct method" and the "adjoint method". In the former method the sensitivity equations have been obtained by direct differentiation of the primary flow equation, and in the latter method variational theory is used to formulate an adjoint sensitivity equation. A comparison between the two methods from a computational point of view revealed that when the number of parameters exceeds the number of performance functions, the adjoint method is more efficient than the direct method, otherwise, the direct method is preferable.

Sensitivity theory was used to establish a sensitivity analysis model for general three dimensional transient groundwater flow. The equations of sensitivity was derived in detail in the continuous equation form. Several performance functions, such as the local piezometric head, the Darcy velocity at certain points in the flow domain, the outflux through a boundary etc. have been derived. Three different methods for calculation of the sensitivity coefficient are presented.

The sensitivity equations and the groundwater flow equations were numerically solved by the Galerkin finite element method in the model. A verification exercise of the model was performed for a two-dimensional non-steady state flow problem with an analytical solution found in the literature. Sensitivity coefficients were carried out both numerically with the developed direct method and with the known analytic solution. Very good agreement between the two solutions was obtained.

The developed sensitivity model was applied to three dimensional (axi-symmetric) groundwater flow in a tunnel system, which was supposed to be located at a depth of 500 meters below the ground surface in a four-layered rock formation. In this case, the sensitivity distribution of the piezometric head was calculated with the direct method and the sensitivity of multiple performance functions to perturbations of the permeability were analyzed by using the adjoint method.

The calculation results showed that the peaks of the sensitivity coefficients appear mostly in the area around the tunnel. The piezometric head at the studied points (nodes) was quite sensitive to perturbations of the permeability in the layer where the points were located, but practically insensitive to perturbations of the permeability in the bottom layer. The flux into the tunnel and the velocity performance were mostly sensitive to perturbation of the permeability in the layer next to the top layer, but practically insensitive to perturbation of the permeability in the bottom layer.

1 INTRODUCTION

1.1 Literature Survey

In general, sensitivity analysis implies a study of the sensitivity to disturbances. These disturbances may have a widely different character: they may be small or large; momentary or permanent; they may be related to initial conditions, boundary conditions or to system's parameters. The major objective of sensitivity analysis of simulation models is to determine the changes in the model output resulting from changes in the model input.

The sensitivity theory has been used extensively in many engineering disciplines. It has been applied to the modelling of nuclear reactor design (Lewins, 1964; Oblow, 1978a, 1978b; Williams and Weisbin, 1977; Cacuci et al., 1983), in electrical power network design and optimization (Director and Rohrer, 1969), and atmospheric contaminate modelling (Marchuk, 1986). Alsmiller et Al, (1984) applied adjoint sensitivity theory to investigate importance of various parameters of a liquid supply model. Chen et al.(1974) and Chavent et al. (1975) used an adjoint sensitivity equation of the linear oil flow equation to compute the gradients of a residual objective function in a history matching application. Lasdon et al. (1986) derived sensitivity equations of the nonlinear gas flow equation to determine the sensitivity of the maximum gas production objective function to changes in the pumping rate. Holmberg (1989) used sensitivity theory to the model of ion dynamics and acidification of soil to investigate the relation between the ion exchanges.

Sensitivity theory has also been used in various models of groundwater flow for describing the variability of system solutions in response to changes in the input parameters such as hydraulic conductivity and storativity, initial and boundary conditions, sources or sinks and boundary flux etc. It makes it possible to investigate and analyse the behaviour and structure of a geohydrologic system and to assess the importance of various governing flow parameters to the behaviour of a specific flow problem. Tomavic (1962), Venuri et al. (1969), McCuen (1973) Yukler (1976) and McElwee (1978) introduced sensitivity theory to groundwater flow. They derived the partial differential equations for the sensitivity coefficient by taking the partial derivative of the flow equation with respect to parameters such as transmissivity and storativity. They applied sensitivity analysis to calibrate models and to establish tolerances on transmissivity and storativity for a given tolerance of the error in the hydraulic head and to estimate the variance and confidence intervals for the hydraulic heads.

Sensitivity analysis is one component of uncertainty analysis. The sensitivity of the performance measure to the parameters can be used to assess how the uncertainty of the performance measure is related to the uncertainty of the parameters. Douglas E. Metcalfe et al (1983) employed sensitivity analysis for performance assessment of prospective radioactive waste repositories. The adjoint sensitivity calibration of the regional conceptual groundwater flow model to the measured piezometric data and to the calculated pressures was used to define a local scale boundary condition. Sykes et al.(1985) applied adjoint sensitivity theory a two-dimension model of steady state confined groundwater flow. The sensitivity of two performance measures, local heads and Darcy velocity, for the system parameters were evaluated by using the Galerkin finite element method. Ahlfeld et al. (1988) used sensitivity theory to derive a general relationship for computing the derivatives of an arbitrary function of the simulation outputs with respect to model inputs in designing contaminated groundwater remediation systems.

Sensitivity analysis also is an important means for solving inverse problems or parameter identification and optimization problems. In solving these problems it is a tool for determining the derivatives of a function or sensitivity coefficients that relate the predicted and measured piezometric heads with respect to the hydraulic conductivity of the aquifer. Neuman (1980) and Townles and Wilson (1985) solved parameter estimation problems for transient confined groundwater flow models. They applied sensitivity methods to compute the gradients of the least squares objective functions with respect to the parameters of interest. Carrera and Neuman (1985) included as the parameters the hydraulic conductivities, specific storage, sources, sinks and boundary fluxes, boundary heads, and initial head conditions for the transient case. Sun and Yeh (1985) used the variational method to evaluate sensitivity coefficients for the identification of the parameter structure, using the sensitivity coefficients in the Gauss-Newton algorithm elements of the Jacobian matrix.

The main approaches to sensitivity analysis are either based on perturbation theory or variational theory. These are referred to as "forward sensitivity formalism" and "adjoint sensitivity formalism", respectively by Cacuci (1981). In the former approach the performance measure sensitivity equation is derived by direct differentiating of the primary flow equations. The variational approach involves the evaluations of an arbitrary function (adjoint function) through an adjoint sensitivity equation, which has a form similar to the primary flow equation.

The adjoint method of sensitivity analysis has been used widely in various fields such as petroleum reservoir history matching (Chavent et al, 1975), electrical engineering problem (Director and Rohrer, 1969) and nuclear reactor assessments (Oblow, 1978). In recent years it has been also used in the field of the groundwater flow simulation. The adjoint sensitivity equation can be derived from either the equations of the primary problem or from its numerical discretized equations as well as problems may be considered. Neuman (1980) used an adjoint methodology as part of an aquifer hydrology parameter estimation routine, thus avoiding the time consuming process of trial and error parameter sampling. Sykes (1985) developed the adjoint sensitivity theory for both the continuous and discrete forms of the dimensional steady state flow in a confined aquifer by using finite element method. Carrera and Neuman (1985) and Samper and Neuman (1986) derived both the continuous and discrete adjoint state equations for transient flow.

1.2 Objectives of the Present Study

The objectives of this study are:

- To make a theoretical development of sensitivity analysis of a general physical problem, in order to establish an appropriate mathematical framework for sensitivity analysis of groundwater flow problems.
- To build a sensitivity analysis model for a three dimensional transient groundwater flow and to apply the model to study the behaviour and structure of geohydrologic systems and to assess the importance of various governing flow parameters to the behaviours of a specific flow problem.
- To establish a sensitivity analysis computer model based on a Galerkin finite element numeric scheme.
- To apply the developed model to study a three-dimensional (axi-symmetric) groundwater flow conditions around a tunnel system.

The remaining part of the report is organized as follows.

Section 2 presents the theory for analyzing the sensitivity of a general set of equations describing a physical problem in order to establish an appropriate mathematical framework. A general sensitivity formalism is derived for both the direct derivative method and the adjoint method. Several performance functions, such as local pressure, the Darcy velocity at selected points, outflux or influx through the boundary and the sum of the squares of the differences between predicted and measure values, are treated. Both the direct method and the adjoint sensitivity method for the simulation of transient groundwater flow is developed. The derivation of the primary equations of groundwater flow and the corresponding sensitivity equations are presented in detail.

Section 3 presents the Galerkin finite element form of the flow equation, the adjoint sensitivity equation and the performance functions.

Section 4 presents three different methods for calculation of the sensitivity coefficient, viz. the influence, the direct equation and the adjoint state method.

Section 5 presents a demonstrative sensitivity analysis of the flow conditions around a tunnel system. The sensitivities of local pressures, the Darcy velocity in the vicinity of the tunnel system and the flux into the tunnel system to permeabilities are evaluated and presented in the form of figures and tables.

Section 6 presents the summary and the conclusions from the present study.

Appendix A gives a description of the computer model used for the calculations in the present study.

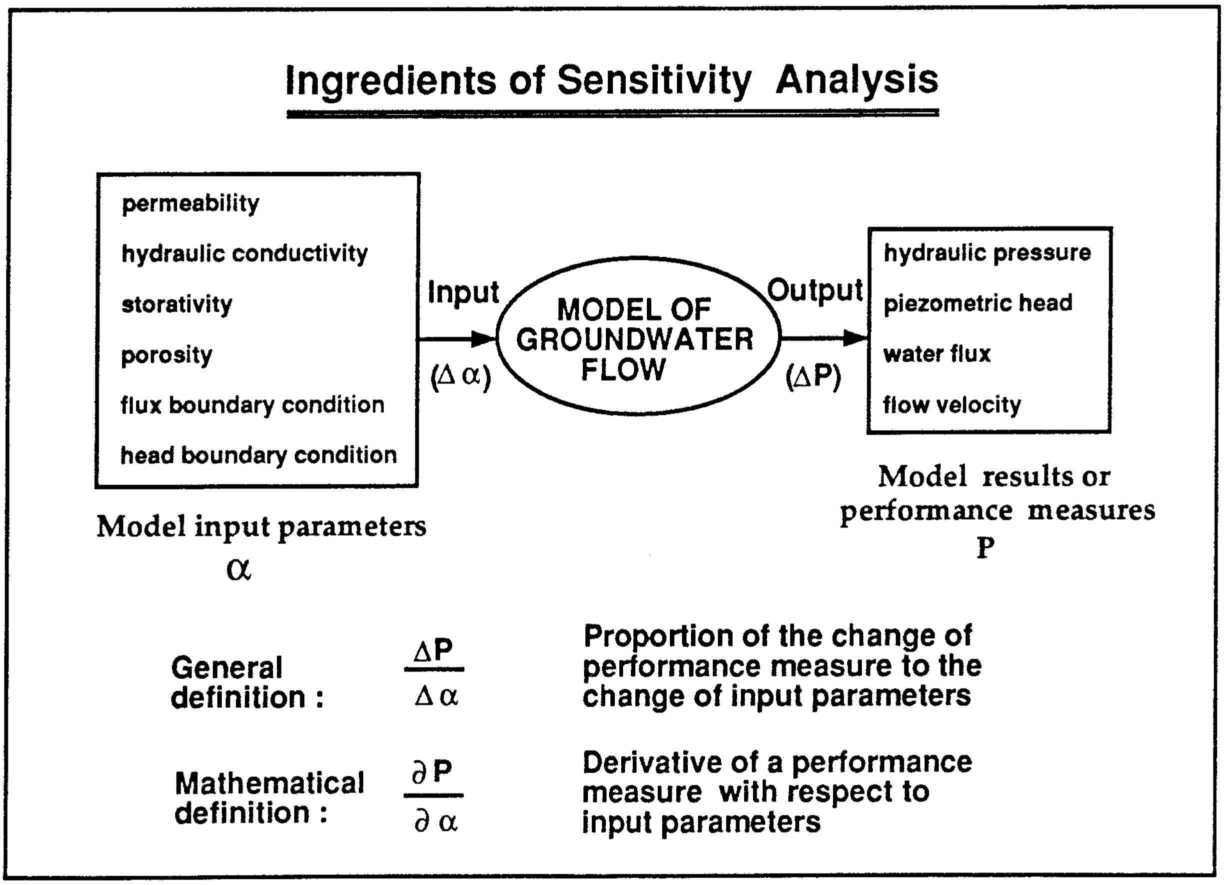
Appendix B presents a verification study of the present sensitivity model for a two-dimensional transient flow problem with an analytical solution found in the literature. The sensitivity coefficients are calculated by the direct method and compared with the analytical solution. The comparisons of the results are shown in figures.

2 MATHEMATICAL STATEMENT OF THE PROBLEM

In general sensitivity analysis is a study of the rate of change in model results (output) to the change in model parameters (input). Thus making it possible to quantify how sensitive the model results are to perturbations in the model parameters. In groundwater flow studies these parameters generally include hydraulic conductivity, permeability, specific storage, porosity, fluxes, boundary and initial conditions. In this section, firstly a general sensitivity theory is presented in order to establish the basic theoretical concepts. Secondly, various performance functions often used in modelling of groundwater flow are regarded. Finally, the sensitivity theory is applied to the modelling of groundwater flow. The continuous adjoint sensitivity equations for 3-dimensional transient flow are derived.

2.1 Definition of Sensitivity

A schematic definition of sensitivity is presented in the following figure:



2.2 General Sensitivity Theory

The general sensitivity theory is applied to many research areas for describing the sensitivity of model outputs to model inputs. The sensitivity equations for the response of a set of general simulation equations, characterized from a physical problem in general, to parameter variation are derived in the sequel.

Firstly, we consider a general system state equation relating the parameters to dependent state variables:

$$V(\{p\},\{\alpha\})=0 \qquad (2-1)$$

where the general system state equation is symbolically represented by V in the previous equation including the appropriate differential equations together with initial and boundary conditions.

where V — vector $(n \times 1)$ of simulation functions (e.g., groundwater flow equation)

$\{p\}$ — vector $(n \times 1)$ of state variables (e.g., pressure)

$\{\alpha\}$ — vector $(m \times 1)$ of all of the parameters in the system (e.g., permeability).

m is the number of components of $\{\alpha\}$ and n is the number of components of $\{p\}$. All of the components in $\{\alpha\}$ for which sensitivity information is sought are independent. We will assume that, for a specific choice of $\{\alpha\}$, a unique solution of equation (2-1) exits and is represented by $\{p\}$. Thus, $\{p\}$ is a function of $\{\alpha\}$, but its dimension is not related to the dimension of $\{\alpha\}$.

Secondly, a specified function of $\{p\}$ and $\{\alpha\}$ is considered and is referred to as a performance function or performance measure by Sykes and Wilson (1985) and as a response function by Oblow (1978). It represents any result of the calculations that is of interest.

$$P=P(\{p\},\{\alpha\}) \qquad (2-2)$$

where $\{p\}$ is a vector $(n \times 1)$ of state variables (e.g., pressure values) and $\{\alpha\}$ is a vector $(m \times 1)$ of system parameters (e.g., permeability, porosity). The performance measure P is a scalar that may be calculated from equation (2-2) using the state variable $\{p\}$ from equation (2-1) for a specified $\{\alpha\}$.

The total sensitivity of performance function with respect to every parameter can be derived using the definition of the total derivative:

$$\frac{dP(\{p\},\{\alpha\})}{d\{\alpha\}^T}=\frac{\partial P(\{p\},\{\alpha\})}{\partial\{\alpha\}^T}+\frac{\partial P(\{p\},\{\alpha\})}{\partial\{p\}^T}\frac{\partial\{p\}}{\partial\{\alpha\}^T} \qquad (2-3)$$

where the superscript T indicates transposition of a vector or a matrix,

$\dfrac{\partial P(\{p\},\{\alpha\})}{\partial\{p\}^T}$ is a matrix of partial derivatives (a Jacobian matrix) with $l \times n$ dimension

and

$\dfrac{\partial\{p\}}{\partial\{\alpha\}^T}$ is a matrix of partial derivatives (a Jacobian matrix) with $n \times m$ dimension.

The equation (2-3) is referred to as *the performance function sensitivity equation*, where $dP/d\{\alpha\}^T$ represents a matrix of total derivatives. The second term on the right hand side of equation (2-3) is a matrix with $l \times m$ dimension. The row dimension of the matrix is equal to the dimension of vector $P(\{p\},\{\alpha\})$ and the column dimension of the matrix is equal to the dimension of vector $\{\alpha\}$.

Similarly, the sensitivity of the performance function to a specific system parameter α_k is determined by differentiating equation (2-2) with respect to it:

$$\frac{dP(\{p\},\{\alpha\})}{d\alpha_k}=\frac{\partial P(\{p\},\{\alpha\})}{\partial\alpha_k}+\frac{\partial P(\{p\},\{\alpha\})}{\partial\{p\}^T}\frac{\partial\{p\}}{\partial\alpha_k} \tag{2-4}$$

For this case $dP/d\alpha_k$ is a vector whose dimension is equal to that of vector P.

Now our problem is how to solve equation (2-3). The gradients of P with respect to the state variables and parameters are readily calculated, since P is explicitly known. Therefore, we focus our attention on solving $\partial\{p\}/\partial\{\alpha\}^T$ which is referred to as *the state sensitivity matrix*, the sensitivity of the state of the system to the parameters.

There are two methods for evaluating $\partial\{p\}/\partial\{\alpha\}^T$. One is to derive a state sensitivity equation in order to obtain directly the state sensitivity matrix $\partial\{p\}/\partial\{\alpha\}^T$. The other is to eliminate $\partial\{p\}/\partial\{\alpha\}^T$ from equation (2-3) by defining *an adjoint sensitivity matrix* $[\psi^*]$ that is obtainable by solving the adjoint sensitivity equation, which will be derived later.

In the first method the state sensitivity equation can be derived by differentiating the system state equation (2-1) with respect to the parameters and we obtain:

$$\frac{\partial V(\{p\},\{\alpha\})}{\partial\{\alpha\}^T}+\frac{\partial V(\{p\},\{\alpha\})}{\partial\{p\}^T}\frac{\partial\{p\}}{\partial\{\alpha\}^T}=0 \tag{2-5}$$

Rewriting the previous equation, we obtain:

$$\frac{\partial\{p\}}{\partial\{\alpha\}^T}=-\left[\frac{\partial V(\{p\},\{\alpha\})}{\partial\{p\}^T}\right]^{-1}\frac{\partial V(\{p\},\{\alpha\})}{\partial\{\alpha\}^T} \tag{2-6}$$

Substituting equation (2-6) into equation (2-3), we obtain:

$$\frac{dP(\{p\},\{\alpha\})}{d\{\alpha\}^T}$$

$$=\frac{\partial P(\{p\},\{\alpha\})}{\partial\{\alpha\}^T}-\frac{\partial P(\{p\},\{\alpha\})}{\partial\{p\}^T}\left[\frac{\partial V(\{p\},\{\alpha\})}{\partial\{p\}^T}\right]^{-1}\frac{\partial V(\{p\},\{\alpha\})}{\partial\{\alpha\}^T} \qquad (2-7)$$

Thus equation (2-7) provides a direct computation of the matrix of total derivatives of performance function P with respect to parameter vector $\{\alpha\}$.

In the second method we multiply equation (2-5) by an arbitrarily defined matrix of function ψ^*, the adjoint state sensitivity matrix $[\psi^*]$ as mentioned above, and add the result to equation (2-3) to obtain:

$$\frac{dP(\{p\},\{\alpha\})}{d\{\alpha\}^T}=\frac{\partial P(\{p\},\{\alpha\})}{\partial\{\alpha\}^T}+\frac{\partial P(\{p\},\{\alpha\})}{\partial\{p\}^T}\frac{\partial\{p\}}{\partial\{\alpha\}^T}$$

$$+[\psi^*]^T\frac{\partial V(\{p\},\{\alpha\})}{\partial\{\alpha\}^T}+[\psi^*]^T\frac{\partial V(\{p\},\{\alpha\})}{\partial\{p\}^T}\frac{\partial\{p\}}{\partial\{\alpha\}^T} \qquad (2-8)$$

Since ψ^* is arbitrary, the terms containing $\partial\{p\}/\partial\{\alpha\}^T$ can be eliminated by letting

$$\frac{\partial P(\{p\},\{\alpha\})}{\partial\{p\}^T}\frac{\partial\{p\}}{\partial\{\alpha\}^T}+[\psi^*]^T\frac{\partial V(\{p\},\{\alpha\})}{\partial\{p\}^T}\frac{\partial\{p\}}{\partial\{\alpha\}^T}=0 \qquad (2-9)$$

Rearranging equation (2-9) we obtain *the adjoint sensitivity equation* as:

$$\left[\frac{\partial V(\{p\},\{\alpha\})}{\partial\{p\}^T}\right]^T[\psi^*]+\left[\frac{\partial P(\{p\},\{\alpha\})}{\partial\{p\}^T}\right]^T=0 \qquad (2-10)$$

Equation (2-8) now can be reduced to:

$$\frac{dP(\{p\},\{\alpha\})}{d\{\alpha\}^T}=\frac{\partial P(\{p\},\{\alpha\})}{\partial\{\alpha\}^T}+[\psi^*]^T\frac{\partial V(\{p\},\{\alpha\})}{\partial\{\alpha\}^T} \qquad (2-11)$$

The sensitivity of performance function is found by substituting the solution of equation (2-10) to equation (2-11), we can obtain the solution of equation (2-11).

The two methods may be summarized as follows:

The first method, usually referred to as the direct method, uses equation (2-3) together with the state sensitivity equation (2-5):

$$\frac{dP(\{p\},\{\alpha\})}{d\{\alpha\}^T}=\frac{\partial P(\{p\},\{\alpha\})}{\partial\{\alpha\}^T}+\frac{\partial P(\{p\},\{\alpha\})}{\partial\{p\}^T}[\psi] \qquad (2-3)$$

$$\frac{\partial V(\{p\},\{\alpha\})}{\partial\{p\}^T}[\psi]+\frac{\partial V(\{p\},\{\alpha\})}{\partial\{\alpha\}^T}=0 \qquad (2-5)$$

where $[\psi] = \partial\{p\}/\partial\{\alpha\}^T$.

The second method, usually referred to as the adjoint method, uses equation (2-11) together with adjoint sensitivity equation (2-10):

$$\frac{dP(\{p\},\{\alpha\})}{d\{\alpha\}^T} = \frac{\partial P(\{p\},\{\alpha\})}{\partial\{\alpha\}^T} + [\psi^*]^T \frac{\partial V(\{p\},\{\alpha\})}{\partial\{\alpha\}^T} \qquad (2-11)$$

$$\left[\frac{\partial V(\{p\},\{\alpha\})}{\partial\{p\}^T}\right]^T [\psi^*] + \left[\frac{\partial P(\{p\},\{\alpha\})}{\partial\{p\}^T}\right]^T = 0 \qquad (2-10)$$

The major computational work involved in computing the performance function sensitivity is in solving the set of linear equations defined by equation (2-5) and equation (2-10), respectively. For equation (2-5) we need to solve $(n \times m)$ systems of linear equations and for equation (2-10) we need to solve $(n \times l)$ systems of linear equations, where m is the number of parameters; n is the number of state variables and l is the number of performance functions. Thus, we may conclude that if the number of parameters exceeds the number of performance functions, then the second method is preferable to the first method. Conversely, if the number of performance functions exceeds the number of parameters then the first method is to be preferred.

In practical uses of sensitivity analysis for groundwater flow, various approaches are chosen according to particular problems of interest in our studies. In the cases, for example, that the sensitivity of the performance measure only on one or a few specific points to multiparameter (i.e., permeability, boundary conditions and initial conditions) is considered and that in parameter identification where the number of parameters to be identified is greater then the number of observation wells, the second method would be advantageous. On the other hand, to avoid instability when data contain noise, the number of parameters to be identified is usually less than the number of observation wells, then the first method may be more efficient. In particular if our interest is directed towards the sensitivity of piezometric heads to a specific system parameter α_k, i.e., in solving equation (2-4), the computational work in using the first method is significantly less than the second method.

2.3 The Performance Function

The performance function defined in equation (2-2) can be any general function of model outputs for which sensitivities are sought. A performance function for sensitivity analysis of groundwater flow may be generally written as:

$$P = \int_T \int_\Omega f(\{\alpha\}, p, t)\, d\Omega\, dt \qquad (2-12)$$

where $f(\{\alpha\},p,t)$ is some unspecified functions of the system state, p is the pressure and $\{\alpha\}$ represents parameters at a time interval.

$\{\alpha\}$ represents a column vector of the system parameters that may be permeability (k), porosity (ϕ), compressibility (c), the recharge or discharge (Q), prescribed head boundary conditions ($\hat{p}$), flux boundary conditions ($\hat{q}$), and initial conditions (p_0) for a transient problem:

$$\{\alpha\}^T = \{k,\phi,c,Q,\hat{p},\hat{q},p_0\} \qquad (2-13)$$

Examples of various forms of $f(\{\alpha\},p,t)$ are:

$$f(\{\alpha\},p,t) = g(x_i,t)p(x_i,t) \qquad (2-14a)$$

$$f(\{\alpha\},p,t) = \sqrt{\sum_{m=1}^{3} q_m^2 \cdot g(x_i,t)} \qquad (2-14b)$$

$$f(\{\alpha\},p,t) = \sum_{n=1}^{m} q_n g(x_i,t) \qquad (2-14c)$$

$$\int_T \int_\Omega f(\{\alpha\},p,t)d\Omega dt = \sum_{t=1}^{T} \sum_{i=1}^{n} [p(x_i,t) - p'(x_i,t]^2 \qquad (2-14d)$$

where x_i is a location vector, $x_i = \{x_1,x_2,x_3\}$.

Equation (2-14a) is used when the performance measure is the pressure at the certain points at a given time t, with $g(x_i,t)$ being an arbitrary weighting function specifying the region and the time of importance. For a particular value of the state variable at location x'_i at time t' the weighting function may be written as below:

$$g(x_i,t) = \delta(x_i - x'_i)\delta(t-t') \qquad (2-15)$$

Where δ is the Dirac function. For steady state case $g(x_i) = \delta(x_i - x_i')$

We may write the performance measure P in matrix form as $P = \{g\}^T\{p\}$, where g denotes dimensionless weights assigned to the selected node points. Weight $g(x_i,t) = 1$ at the node points x'_i at time t' and $g(x_i,t) = 0$ at all other node points and all other time level. So for this performance measure the second term of the adjoint sensitivity equation (2-10) becomes:

$$\left[\frac{\partial P}{\partial \{p\}^T}\right]^T = \frac{\partial P}{\partial \{p\}} = \{g\} \qquad (2-16)$$

which is independent of the pressures $\{p\}$. The first term at the right side of equation (2-11) becomes:

$$\frac{\partial P}{\partial\{\alpha\}^T} = \frac{\partial\{g\}^T}{\partial\{\alpha\}^T}\{p\} = 0 \qquad t = t' \qquad (2-17)$$

since $\partial g_i/\partial\alpha_k = 0$. In this case the direct sensitivity effect term, viz. the first term of performance function sensitivity equation (2-3) or equation (2-11) is zero.

In some problems we may consider the magnitude of the Darcy velocity at a selected point as a performance function using equation (2-14b) as a function of the system state. $P = \sqrt{\sum_{m=1}^{3} q_m^2}$ is the magnitude of the Darcy velocity at a point x_i' in the domain. For this case the performance measure P is a function of the hydraulic conductivity and the gradient of the state variables of pressure (Sykes et.al, 1985), since $q_1 = K_{11}\partial p/\partial x_1$, $q_2 = K_{22}\partial p/\partial x_2$ and $q_3 = K_{33}\partial p/\partial x_3$.

In some studies we may be interested in the flow rate through a certain region or a specific boundary. Then equation (2-14c) may be considered. For this case the performance function P becomes the sum of the outflux or influx through a boundary, where x'_i indicates the location of the nodes on the boundary and q_n is the normal flux through the boundary.

Equation (2-14d) may be considered a general optimization function given as the sum of the squares of the differences between predicted and measured (p') pressure values over the time interval. Performance functions of the form of equation (2-14d) are commonly used in parameter estimation problems, for example when the minimum residual formulation and the Gauss-Newton algorithm are used (Neuman, et.al, 1980 and Yeh, W.W-G., 1986).

The performance measure of interest in contaminate transport problems is often the mass discharge and P is a function of both the fluid flux and species concentration (David P. Ahlfeld et.al, 1988). The theory presented here can be used to derive performance measures of interest in thermal, mechanical, flow, or mass transport processes in which the sensitivity of a selected performance measure can be determined with respect to any system parameter of interest.

2.4 Sensitivity Analysis of Groundwater Flow

In section 2.1 the sensitivity equations for general simulation equation to parameter variation have been derived. This section deals with the development of both continuous adjoint sensitivity equations and direct sensitivity equations for a three-dimensional transient groundwater flow model (R. Thunvik and C. Braester, 1988).

2.4.1 Groundwater flow equation (primary problem)

We substitute Darcy's law as following form:

$$q_i = -\frac{k_{ij}}{\mu}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right) \qquad (2-18a)$$

into the continuity equation. Then the governing equation for three dimensional transient flow is obtained as following:

$$\phi\rho c\frac{\partial p}{\partial t} - \frac{\partial}{\partial x_i}\left[\rho\frac{k_{ij}}{\mu}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right)\right] + Q = 0 \quad i = 1,2,3 \qquad (2-18b)$$

The initial and boundary conditions associated with equation (2-18) are:

$$p(\Omega, 0) = p_0 \qquad \in \Omega, t = 0 \qquad (2-19a)$$

$$p(\Gamma_1, t) = \hat{p} \qquad \in \Gamma_1 \qquad (2-19a)$$

$$-\frac{k_{ij}}{\mu}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right)n_i = \hat{q} \qquad \in \Gamma_2 \qquad (2-19b)$$

In case that the initial conditions are unknown, we assume that the system is initially at steady state. In case that the initial condition required by equation (2-18) are determined from the steady state flow equation as below:

$$-\frac{\partial}{\partial x_i}\left[\rho\frac{k_{ij}}{\mu}\left(\frac{\partial p_0}{\partial x_j} - \rho g_j\right)\right] + Q = 0 \qquad i = 1,2,3 \qquad (2-20)$$

with the boundary conditions:

$$p_0(\Gamma_1) = \hat{p}_0 \qquad \in \Gamma_1 \qquad (2-21a)$$

$$-\frac{k_{ij}}{\mu}\left(\frac{\partial p_0}{\partial x_j} - \rho g_j\right)n_i = \hat{q}_0 \qquad \in \Gamma_2 \qquad (2-21b)$$

where c is the total compressibility $(c^f + c^r)$, c^f is the compressibility of the fluid, c^r is the compressibility of the rock, $\hat{p}$ denotes prescribed values of pressure on boundary Γ_1, $\hat{q}$ denotes prescribed flux normal to boundary Γ_2 (as designated by the components of the unit inward normal), n_i is an inward normal vector, $\Gamma = \Gamma_1 + \Gamma_2$ represents the external boundary of the spatial domain Ω governed by equation (2-18a), p_0 is the initial pressure over the domain Ω, $\hat{p}_0$ and $\hat{q}_0$ are prescribed values of the pressure and prescribed flux on the boundary at steady state, respectively.

The pressures are obtained by solving equation (2-18a) with equations from (2-19) to (2-21). These equations describe the so-called *primary problem.*

2.4.2 Direct sensitivity analysis

The sensitivity of the performance function P which was defined by equation (2-12) to the changes of any specific parameter α_k is:

$$\frac{\partial P}{\partial \alpha_k}=\int_T\int_\Omega\left[\frac{\partial f(\{\alpha\},p,t)\,|_p}{\partial \alpha_k}+\frac{\partial f(\{\alpha\},p,t)\,|_{\{\alpha\}}}{\partial p}\psi\right]d\Omega dt \qquad (2-22)$$

where $\psi=\partial p/\partial\alpha_k$ is the sensitivity of the pressure (p) to parameter α_k and is referred to as *the state sensitivity*. Equation (2-22) is referred to as *the performance measure marginal sensitivity* (Sykes 1985).

The state sensitivity can be calculated by solving the state sensitivity equation, which can be obtained by differentiating equation (2-18a) with respect to α_k as follows below:

$$\frac{\partial}{\partial x_i}\left[\frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\partial\alpha_k}\left(\frac{\partial p}{\partial x_j}-\rho g_j\right)+\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial\psi}{\partial x_j}\right]-\frac{\partial Q}{\partial\alpha_k}=\frac{\partial(\phi\rho c)}{\partial\alpha_k}\frac{\partial p}{\partial t}+(\phi\rho c)\frac{\partial\psi}{\partial t} \qquad (2-23)$$

The boundary conditions associated with equation (2-23) are:

$$\psi(\Gamma_1)=0 \qquad \in\Gamma_1 \qquad (2-24a)$$

$$-\frac{\partial\left(\frac{k_{ij}}{\mu}\right)}{\partial\alpha_k}\left(\frac{\partial p}{\partial x_j}-\rho g_j\right)n_i-\left(\frac{k_{ij}}{\mu}\right)\frac{\partial\psi}{\partial x_j}n_i=\frac{\partial\hat{q}}{\partial\alpha_k} \qquad \in\Gamma_2 \qquad (2-24b)$$

In equation (2-23), the first and third terms of the left hand side and the first term in the right hand side are known through the solution of equation (2-18) and (2-19). The known terms are defined as:

$$D=\frac{\partial Q}{\partial\alpha_k}-\frac{\partial}{\partial x_i}\left[\frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\partial\alpha_k}\left(\frac{\partial p}{\partial x_j}-\rho g_j\right)\right]+\frac{\partial(\phi\rho c)}{\partial\alpha_k}\frac{\partial p}{\partial t} \qquad (2-25)$$

Substitution of equation (2-25) into equation (2-23) yields:

$$(\phi\rho c)\frac{\partial\psi}{\partial t}-\frac{\partial}{\partial x_i}\left[\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial\psi}{\partial x_j}\right]+D=0 \qquad (2-26)$$

Equation (2-26) is referred to as *the state sensitivity equation*. Solution of Equation (2-26) with the boundary conditions (2-24) gives a direct measure of the state sensitivities. If the state sensitivity ψ is desired for each point in the domain then equation (2-26) with boundary conditions (2-24) must be solved.

For steady state flow conditions the state sensitivity equation becomes:

$$-\frac{\partial}{\partial x_i}\left[\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial \psi_0}{\partial x_j}\right]+D_0=0 \qquad (2-27)$$

where D_0 is:

$$D_0=\frac{\partial Q}{\partial \alpha_k}-\frac{\partial}{\partial x_i}\left[\frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\partial \alpha_k}\left(\frac{\partial p_0}{\partial x_j}-\rho g_j\right)\right] \qquad (2-28)$$

and the boundary conditions are:

$$\psi_0(\Gamma_1)=0 \qquad \in \Gamma_1 \qquad (2-29a)$$

$$-\frac{\partial\left(\frac{k_{ij}}{\mu}\right)}{\partial \alpha_k}\left(\frac{\partial p_0}{\partial x_j}-\rho g_j\right)n_i-\left(\frac{k_{ij}}{\mu}\right)\frac{\partial \psi_0}{\partial x_j}n_i=\frac{\partial \hat{q}_0}{\partial \alpha_k} \qquad \in \Gamma_2 \qquad (2-29b)$$

The sensitivity of the performance function can be obtained from equation (2-22) together with the state sensitivity equation (2-26). This method of obtaining the state sensitivity is referred to as the direct sensitivity method.

2.4.3 Adjoint sensitivity analysis

Firstly the derivation of the adjoint equation is made. Multiplying equation (2-26) by an arbitrary differentiable function ψ^* and integrating over space Ω and over time T, we obtain:

$$\int_T\int_\Omega\left\{\psi^*(\phi\rho c)\frac{\partial \psi}{\partial t}-\psi^*\frac{\partial}{\partial x_i}\left[\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial \psi}{\partial x_j}+\psi^* D\right]\right\}d\Omega\, dt=0 \qquad (2-30)$$

For steady state we obtain:

$$\int_\Omega\left\{-\psi_0^*\frac{\partial}{\partial x_i}\left[\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial \psi_0}{\partial x_j}+\psi_0^* D_0\right]\right\}d\Omega=0 \qquad (2-31)$$

Applying Green's theorem to the second term of equation (2-30) and the first of the equation (2-31), respectively, we obtain:

$$\int_T\int_\Omega \psi^*\frac{\partial}{\partial x_i}\left[\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial \psi}{\partial x_j}\right]d\Omega dt$$

$$=\int_T\int_\Omega \psi\frac{\partial}{\partial x_j}\left[\left(\rho\frac{k_{ji}}{\mu}\right)\frac{\partial \psi^*}{\partial x_i}\right]d\Omega dt$$

$$+\int_T\int_\Gamma \psi\left(\rho\frac{k_{ji}}{\mu}\right)\frac{\partial \psi^*}{\partial x_i}n_j d\Gamma dt-\int_T\int_\Gamma \psi^*\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial \psi}{\partial x_j}n_i d\Gamma dt \qquad (2-32)$$

for transient flow and

$$\int_{\Omega} \psi_0^* \frac{\partial}{\partial x_i}\left[\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial \psi_0}{\partial x_j}\right] d\Omega$$

$$= \int_{\Omega} \psi_0 \frac{\partial}{\partial x_j}\left[\left(\rho\frac{k_{ji}}{\mu}\right)\frac{\partial \psi_0^*}{\partial x_i}\right] d\Omega$$

$$+ \int_{\Gamma} \psi_0\left(\rho\frac{k_{ji}}{\mu}\right)\frac{\partial \psi_0^*}{\partial x_i} n_j d\Gamma - \int_{\Gamma} \psi_0^*\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial \psi_0}{\partial x_j} n_i d\Gamma \qquad (2-33)$$

for steady state flow, respectively, where $k_{ij} = k_{ji}$.

Applying Green's theorem to the third term of equation (2-30) and the second term of equation (2-33), respectively, we obtain:

$$\int_{T}\int_{\Omega} \psi^* D \, d\Omega dt$$

$$= \int_{T}\int_{\Omega} \psi^* \frac{\partial Q}{\partial \alpha_k} d\Omega dt - \int_{T}\int_{\Omega} \frac{\partial \psi^*}{\partial x_i} \frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\partial \alpha_k}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right) d\Omega dt$$

$$- \int_{T}\int_{\Gamma} \psi^* \frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\partial \alpha_k}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right) n_i d\Gamma dt$$

$$+ \int_{T}\int_{\Omega} \psi^* \frac{\partial(\phi\rho c)}{\partial \alpha_k}\frac{\partial p}{\partial t} d\Omega dt \qquad (2-34)$$

for transient flow and

$$\int_{\Omega} \psi_0^* D_0 d\Omega$$

$$= \int_{\Omega} \psi_0^* \frac{\partial Q}{\partial \alpha_k} d\Omega - \int_{\Omega} \frac{\partial \psi_0^*}{\partial x_i} \frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\partial \alpha_k}\left(\frac{\partial p_0}{\partial x_j} - \rho g_j\right) d\Omega$$

$$- \int_{\Gamma} \psi_0^* \frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\partial \alpha_k}\left(\frac{\partial p_0}{\partial x_j} - \rho g_j\right) n_i d\Gamma \qquad (2-35)$$

for steady state flow, respectively, where τ is the final time on the time interval.

The first term of equation (2-30) can be derived as below:

$$\int_T \int_\Omega \psi^*(\phi\rho c)\frac{\partial\psi}{\partial t}d\Omega dt$$

$$= \int_T \int_\Omega (\phi\rho c)\frac{\partial(\psi^*\psi)}{\partial t}d\Omega dt - \int_T \int_\Omega (\phi\rho c)\frac{\partial\psi^*}{\partial t}\psi d\Omega dt$$

$$= \int_\Omega (\phi\rho c)\,[\psi^*(\tau)\psi(\tau) - \psi^*(0)\psi(0)]\,d\Omega - \int_T \int_\Omega (\phi\rho c)\frac{\partial\psi^*}{\partial t}\psi d\Omega dt \qquad (2-36)$$

Adding these expanded terms of equation (2-30) and equation (2-31) to the performance measure marginal sensitivity (2-22), it becomes:

$$\frac{\partial P}{\partial\alpha_k} = \int_T \int_\Omega \left[\frac{\partial f(\{\alpha\},p)\,|_p}{\partial\alpha_k} + \psi^*\frac{\partial(\phi\rho c)}{\partial\alpha_k}\frac{\partial p}{\partial t} + \psi^*\frac{\partial Q}{\partial\alpha_k} - \frac{\partial\psi^*}{\partial x_i}\frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\partial\alpha_k}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right)\right]d\Omega dt$$

$$- \int_T \int_{\Gamma_1} \frac{\partial\hat{p}}{\partial\alpha_k}\left(\rho\frac{k_{ji}}{\mu}\frac{\partial\psi^*}{\partial x_j}\right)n_j d\Gamma_1 dt - \int_T \int_{\Gamma_2} \psi^*\frac{\partial\hat{q}}{\partial\alpha_k}d\Gamma_2 dt$$

$$+ \int_\Omega \left[\psi_0^*\frac{\partial Q}{\partial\alpha_k} - \frac{\partial\psi_0^*}{\partial x_i}\frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\partial\alpha_k}\left(\frac{\partial p_0}{\partial x_j} - \rho g_j\right)\right]d\Omega$$

$$- \int_{\Gamma_1} \frac{\partial\hat{p}_0}{\partial\alpha_k}\left(\rho\frac{k_{ji}}{\mu}\frac{\partial\psi_0^*}{\partial x_j}\right)n_j d\Gamma_1 - \int_{\Gamma_2} \psi_0^*\frac{\partial\hat{q}_0}{\partial\alpha_k}d\Gamma_2 + H \qquad (2-37)$$

where

$$H = \int_T \int_\Omega \left[\frac{\partial f(\{\alpha\},p)\,|_{\{\alpha\}}}{\partial p}\psi - \psi\frac{\partial}{\partial x_j}\left[\left(\rho\frac{k_{ji}}{\mu}\right)\frac{\partial\psi^*}{\partial x_i}\right] + (\phi\rho c)\psi\frac{\partial\psi^*}{\partial t}\right]d\Omega dt$$

$$+ \int_T \int_\Gamma \left[-\psi\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial\psi^*}{\partial x_i}n_j + \psi^*\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial\psi}{\partial x_j}n_i - \psi^*\frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\alpha_k}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right)n_i\right]d\Gamma dt$$

$$+ \int_\Gamma \left[-\psi_0\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial\psi_0^*}{\partial x_i}n_j + \psi_0^*\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial\psi_0}{\partial x_j}n_i - \psi_0^*\frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\alpha_k}\left(\frac{\partial p_0}{\partial x_j} - \rho g_j\right)n_i\right]d\Gamma$$

$$+ \int_\Omega -\psi_0\frac{\partial}{\partial x_j}\left(\rho\frac{k_{ji}}{\mu}\frac{\partial\psi_0^*}{\partial x_i}\right)d\Omega$$

$$- \int_\Omega [(\phi\rho c)\psi^*(\tau)\psi(\tau) - (\phi\rho c)\psi^*(0)\psi(0)]\,d\Omega \qquad (2-38)$$

To eliminate the unknown state sensitivities ψ and ψ_0 in equation (2-37), we define ψ^* and ψ_0^* such that H=0. Letting the first integrand in equation (3-38) be equal to zero, we obtain:

$$(\phi\rho c)\frac{\partial\psi^*}{\partial t}-\frac{\partial}{\partial x_j}\left[\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial\psi^*}{\partial x_i}\right]+\frac{\partial f(\{\alpha\},p)}{\partial p}=0 \qquad (2-39)$$

The second integrand which is integrated on the boundary may be rewritten by substitution of equation (2-19) and (2-24) and we obtain:

$$\int_T\int_\Gamma\left[-\psi\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial\psi^*}{\partial x_i}n_j+\psi^*\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial\psi}{\partial x_j}n_i-\psi^*\frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\alpha_k}\left(\frac{\partial p}{\partial x_j}-\rho g_j\right)n_i\right]d\Gamma dt$$

$$=-\int_T\int_\Gamma\left[\psi\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial\psi^*}{\partial x_i}n_j+\psi^*\frac{\partial\hat{q}}{\partial\alpha_k}\right]d\Gamma dt \qquad (2-40)$$

In order to eliminate equation (2-40) the boundary conditions may be defined for equation (2-39) as below:

$$\psi^*(\Gamma_1,t)=0 \qquad \in\Gamma_1 \qquad (2-41a)$$

$$\frac{k_{ji}}{\mu}\frac{\partial\psi^*}{\partial x_i}n_j=0 \qquad \in\Gamma_2 \qquad (2-41b)$$

From the first term of the last integrand in equation (2-38) we may define the terminal condition of equation (2-39) as:

$$\psi^*(\Omega,\tau)=0 \qquad \in\Omega, t=\tau \qquad (2-42)$$

So far we have obtained the adjoint problem that is described by *the adjoint state sensitivity equation:*

$$(\phi\rho c)\frac{\partial\psi^*}{\partial t}-\frac{\partial}{\partial x_j}\left[\left(\rho\frac{k_{ji}}{\mu}\right)\frac{\partial\psi^*}{\partial x_i}\right]+\frac{\partial f(\{\alpha\},p)}{\partial p}=0 \qquad (2-39)$$

$$\psi^*(\Gamma_1,t)=0 \qquad \in\Gamma_1 \qquad (2-41a)$$

$$\frac{k_{ji}}{\mu}\frac{\partial\psi^*}{\partial x_i}n_j=0 \qquad \in\Gamma_2 \qquad (2-41b)$$

$$\psi^*(\Omega,\tau)=0 \qquad \in\Omega, t=\tau \qquad (2-42)$$

in which the arbitrary function ψ^* is chosen to satisfy the above equation and conditions. The arbitrary function ψ^* is called adjoint state.

The adjoint state value ψ_0^* in steady state can be evaluated by following equations which are obtained by using the similar treatment as the transient case:

$$(\phi\rho c)\psi^*(0)-\frac{\partial}{\partial x_j}\left[\left(\rho\frac{k_{ji}}{\mu}\right)\frac{\partial\psi_0^*}{\partial x_i}\right]+\frac{\partial f(\{\alpha\},p_0)}{\partial p_0}=0 \qquad (2-43)$$

$$\psi_0^*(\Gamma_1)=0 \qquad \in\Gamma_1 \qquad (2-44a)$$

$$\frac{k_{ji}}{\mu}\frac{\partial\psi_0^*}{\partial x_i}n_j=0 \qquad \in\Gamma_2 \qquad (2-44b)$$

The adjoint state variable at t=0, $\psi^*(0)$ is considered a component in the source term to determine the steady state adjoint state value ψ_0^*.

Comparing the equation (2-18a) for the primary problem and the adjoint sensitivity equation the only difference between them is that there are different values in their third terms. This implies that only a small modification in the computer code for the primary problem is needed in order to solve the adjoint problem. It is notable that the adjoint problem is reversed in time as compared to the primary problem.

Since the adjoint state equation has been defined to set H=0, the equation (2-37) can be simplified to:

$$\begin{aligned}\frac{\partial P}{\partial\alpha_k}=&\int_T\int_\Omega\left[\frac{\partial f(\{\alpha\},p)\,|_p}{\partial\alpha_k}+\psi^*\frac{\partial(\phi\rho c)}{\partial\alpha_k}\frac{\partial p}{\partial t}+\psi^*\frac{\partial Q}{\partial\alpha_k}-\frac{\partial\psi^*}{\partial x_i}\frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\partial\alpha_k}\left(\frac{\partial p}{\partial x_j}-\rho g_j\right)\right]d\Omega dt\\&-\int_T\int_{\Gamma_1}\frac{\partial\hat{p}}{\partial\alpha_k}\left(\rho\frac{k_{ji}}{\mu}\frac{\partial\psi^*}{\partial x_j}\right)n_j d\Gamma_1 dt-\int_T\int_{\Gamma_2}\psi^*\frac{\partial\hat{q}}{\partial\alpha_k}d\Gamma_2 dt\\&+\int_\Omega\left[\psi_0^*\frac{\partial Q}{\partial\alpha_k}-\frac{\partial\psi_0^*}{\partial x_i}\frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\partial\alpha_k}\left(\frac{\partial p_0}{\partial x_j}-\rho g_j\right)\right]d\Omega\\&-\int_{\Gamma_1}\frac{\partial\hat{p}_0}{\partial\alpha_k}\left(\rho\frac{k_{ji}}{\mu}\frac{\partial\psi_0^*}{\partial x_j}\right)n_j d\Gamma_1-\int_{\Gamma_2}\psi_0^*\frac{\partial\hat{q}_0}{\partial\alpha_k}d\Gamma_2\end{aligned} \qquad (2-45)$$

in which all terms are known. The pressure values p are obtained from the solution of the primary equation, and the adjoint states ψ^* and its initial values are obtained from the solutions of the adjoint state equations.

The first term in equation (2-45) represents the direct sensitivity effect of α_k on the performance function. The remaining five terms represent the transient contributions to the marginal sensitivity associated with porosity, compressibility and density, recharge or discharge, permeability, prescribed pressure and prescribed boundary fluxes, respectively. The last four terms represent the contributions from the initial conditions.

3 METHOD OF SOLUTION

Practical application of sensitivity theory is general limited to simulation models defined by systems of algebraic equations. So it is necessary and useful for practical modelling that the sensitivity equation is derived to the algebraic simulation equations of the original differential equations by numerical discretization. In this chapter, we derive the sensitivity equations in a discretized form using the Galerkin finite element method.

3.1 Numerical Solution of the Flow Equation

The primary flow problem defined by equation (2-18) to (2-21) is generally solved with discrete numerical techniques. For a discretization system of n nodes, in which l nodes are prescribed, this would results a linear matrix equation of the form:

$$[A(\phi,\rho,c)]\left\{\frac{dp}{dt}\right\} - [B(\rho,k,\mu)]\,\{p\} = \{R_p(\{\alpha^*\})\} \qquad (3-1)$$

where $\{\alpha^*\}^T = \{Q,\hat{p},\hat{q},\hat{p}_0,\hat{q}_0\}$, [A] and [B] are the coefficient matrices with $(n\text{-}l)$ rows, {p} represents the vector of $(n\text{-}l)$ unknown nodal pressure, and $\{R_p\}$ is the source term including the effects of recharge-discharge Q and boundary conditions.

Variables p in the flow problem are approximated in terms of the pressure by

$$p = \{N\}^T\{p\} \qquad (3-2)$$

where {N} is a vector of trial functions. The individual terms of the coefficient matrices [A], [B] and the source term vector $\{R_p\}$ are:

$$a_{IJ} = \int_\Omega (\phi\rho c) N_I N_J \, d\Omega \qquad (3-3)$$

$$b_{IJ} = \int_\Omega \rho \frac{k_{ij}}{\mu}\frac{\partial N_I}{\partial x_i}\frac{\partial N_J}{\partial x_j}\, d\Omega \qquad (3-4)$$

$$r_{p,I} = \int_\Omega N_I Q_a \, d\Omega + \int_\Omega \rho\frac{k_{ij}}{\mu}\rho g_i N_{I,i}\, d\Omega + \int_{\Gamma_2} N_I \hat{q}\, d\Gamma_2 + \sum_{p=1}^{n} Q_p \delta(x_i - x_p) - \sum_{J=1}^{L} b_{IJ}\hat{p}_J \qquad (3-5)$$

at initial time equation (3-5) becomes:

$$r_{p,I} = \int_\Omega N_I Q_a \, d\Omega + \int_\Omega \rho\frac{k_{ij}}{\mu}\rho g_i N_{I,i}\, d\Omega + \int_{\Gamma_2} N_I \hat{q}_0\, d\Gamma_2 + \sum_{p=1}^{n} Q_p \delta(x_i - x_p) - \sum_{J=1}^{L} b_{IJ}\hat{p}_{0J} \qquad (3-6)$$

in which I, J are matrix row and column indices and i, j are spatial coordinate indices. Q_a is the regional source and Q_p is the point source assigned to individual node points x_p of the discretized domain. The source term of equation (3-1) represents the contributions from boundary flux, sources and prescribed pressure boundary, respectively.

3.2 Numerical Solution of the Sensitivity Equations

The performance measure for a spatial discrete system is defined as:

$$P = \int_T F(\{\alpha\},\{p\})dt \tag{3-7}$$

where $\{\alpha\}$ is a vector of numerical model parameters which may include element permeabilities and storativities, nodal point fluxes, and prescribed pressure nodes and $\{p\}$ is the vector of pressure in the spatial discrete system and it is a function of time.

3.2.1 Direct sensitivity equations

Differentiation of the performance function (3-7) and equation (3-1) with respect to a parameter α_k yields:

$$\frac{\partial P}{\partial \alpha_k} = \int_T \left[\frac{\partial F(\{\alpha\},\{p\})\,|_{\{p\}}}{\partial \alpha_k} + \frac{\partial F(\{\alpha\},\{p\})\,|_{\{\alpha\}}}{\partial \{p\}^T} \{\psi_k\} \right] dt \tag{3-8}$$

where $\{\psi_k\} = \partial\{p\}/\partial\alpha_k$ and

$$\frac{\partial [A]}{\partial \alpha_k}\frac{\partial \{p\}}{\partial t} + [A]\frac{\partial \{\psi_k\}}{\partial t} - \frac{\partial [B]}{\partial \alpha_k}\{p\} - [B]\,\{\psi_k\} = \frac{\partial \{R_p\}}{\partial \alpha_k} \tag{3-9}$$

The above equation can be shortened to

$$[A]\left\{\frac{d\psi_k}{dt}\right\} - [B]\,\{\psi_k\} = \{R_\psi(\{\alpha\},\{p\})\} \tag{3-10}$$

where

$$\{R_\psi\} = \frac{\partial \{R_p\}}{\partial \alpha_k} - \frac{\partial [A]}{\partial \alpha_k}\left\{\frac{dp}{dt}\right\} + \frac{\partial [B]}{\partial \alpha_k}\{p\} \tag{3-11}$$

$\{\psi_k\}$ is the state sensitivity vector which expresses the sensitivity of {p} to the *k*th parameter and is obtained by solving equation (3-10). The sensitivity of performance measure can be obtained by solving equation (3-8) with the result from equation (3-10). Equation (3-10) is the sensitivity state equation in discrete form. We use backward finite difference approximation for the time derivatives of equation (3-10) to obtain:

$$\left[\frac{A}{\Delta t}-B\right]^{t_i}\{\psi_k\}^{t_i}+\left[\frac{-A}{\Delta t}\right]^{t_i}\{\psi_k\}^{t_{i-1}}=\{R_\psi\}^{t_i} \tag{3-12}$$

Equation (3-12) is a set of linear algebraic equations. It may be expressed in a matrix form as follows:

$$\begin{bmatrix} [D^{t_1}] & 0 & 0 & 0 & 0 \\ [C^{t_2}] & [D^{t_2}] & 0 & 0 & 0 \\ 0 & [C^{t_3}] & [D^{t_3}] & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & [C^{t_n}] & [D^{t_n}] \end{bmatrix} \begin{Bmatrix} \{\psi_k\}^{t_1} \\ \{\psi_k\}^{t_2} \\ \{\psi_k\}^{t_3} \\ \cdot \\ \{\psi_k\}^{t_n} \end{Bmatrix} = \begin{Bmatrix} \{R_\psi\}^{t_1}-[C^{t_1}]\{\psi_k\}^{0} \\ \{R_\psi\}^{t_2} \\ \{R_\psi\}^{t_3} \\ \cdot \\ \{R_\psi\}^{t_n} \end{Bmatrix} \tag{3-13}$$

where $[D^{t_i}]$ represents $[A/\Delta t - B]^{t_i}$ and $[C^{t_i}]$ represents $[-A/\Delta t]^{t_i}$ at corresponding time level. The superscript t_i indicate the different time level. For convenience equation (3-13) is simplified in the below form:

$$[\mathcal{A}]\{\Psi_k\}=\{\mathcal{R}_\psi\} \tag{3-14}$$

$[\mathcal{A}]$ represent the global coefficient matrix in equation (3-13).

$$\{\Psi_k\}^T=\left\{\{\psi_k\}^{t_1},\{\psi_k\}^{t_2},\cdots,\{\psi_k\}^{t_n}\right\} \tag{3-15a}$$

$$\{\mathcal{R}_\psi\}^T=\left\{\{R_\psi\}^{t_1}-[C]^{t_1}\{\psi_k\}^{0},\{R_\psi\}^{t_2},\cdots,\{R_\psi\}^{t_n}\right\} \tag{3-15b}$$

where $\{\psi_k\}^0$ is the state sensitivity vector at time = 0.

3.2.2 Adjoint sensitivity equations

Multiplying equation (3-14) by the arbitrary constant vector $\{\Psi^*\}$ and adding the result to equation (3-8) gives the marginal performance sensitivity:

$$\frac{\partial P}{\partial \alpha_k}=\int_T\left\{\frac{\partial F(\{\alpha\},\{p\})\,|_{\{p\}}}{\partial \alpha_k}+\left[\frac{\partial F(\{\alpha\},\{p\})\,|_{\{\alpha\}}}{\partial\{p\}}\right]^T\{\Psi_k\}\right\}dt$$

$$+\int_T\left\{-\{\Psi^*\}^T[\mathcal{A}]\{\Psi_k\}+\{\Psi^*\}^T\{\mathcal{R}_\psi\}\right\}dt \tag{3-16}$$

Since the vector $\{\Psi^*\}$ is arbitrary, then the terms containing $\{\Psi_k\}$ in the above equation can be eliminated by letting

$$\{\Psi_k\}^T\left[\frac{\partial F(\{\alpha\},\{p\})}{\partial\{p\}}\right]-\{\Psi_k\}^T[\mathcal{A}]^T\{\Psi^*\}=0 \qquad (3-17)$$

After eliminate on of $\{\Psi_k\}$, equation (3-17) may be written in matrix form as:

$$\begin{bmatrix} [D^{t_1}]^T & [C^{t_2}]^T & 0 & 0 & 0 \\ 0 & [D^{t_2}]^T & [C^{t_3}]^T & 0 & 0 \\ 0 & 0 & [D^{t_3}]^T & [C^{t_4}]^T & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & [D^{t_\tau}]^T \end{bmatrix} \begin{Bmatrix} \{\psi^*\}^0 \\ \{\psi^*\}^{t_1} \\ \{\psi^*\}^{t_2} \\ \cdot \\ \{\psi^*\}^{t_{\tau-1}} \end{Bmatrix} = \begin{Bmatrix} \partial F/\partial\{p\}^{t_0} \\ \partial F/\partial\{p\}^{t_1} \\ \partial F/\partial\{p\}^{t_2} \\ \cdot \\ \partial F/\partial\{p\}^{t_{\tau-1}} \end{Bmatrix} \qquad (3-18)$$

The above matrix equation may be written as:

$$[D^{t_i}]^T\{\psi^*\}^{t_{i-1}}+[C^{t_i}]^T\{\psi^*\}^{t_i}=\left\{\frac{\partial F}{\partial\{p\}^{t_{i-1}}}\right\} \qquad i=1,2,\ldots,\tau \qquad (3-19)$$

Substituting the definition of [D] and [C] into equation (3-19), we obtain the algebraic form of the adjoint equation:

$$[A]^T\left\{\frac{d\psi^*}{dt}\right\}-[B]^T\{\psi^*\}=\left\{\frac{\partial F}{\partial\{p\}}\right\} \qquad (3-20)$$

with the condition $\{\psi^*\}^{t_\tau}=0$ at terminal time, where $[A]^T$ and $[B]^T$ are the transposed [A] and [B] which the individual terms are given by equation (3-3) and (3-4), respectively. $\{\psi^*\}$ is the nodal values of the adjoint state. The term on the right hand side may be written as

$$\frac{\partial F}{\partial\{p\}}=\frac{\partial}{\partial\{p\}}\int_\Omega f(\{\alpha\},p)d\Omega=\int_\Omega\left(\frac{\partial f}{\partial p}\right)N_I d\Omega \qquad (3-21)$$

Letting us review equation (3-18), we can clearly see that the expanded matrix equation (3-18) is resulted from using backward finite difference approximation reversely for the time derivative in the adjoint equation (3-20).

The marginal performance sensitivity can be simplified to

$$\frac{\partial P}{\partial\alpha_k}=\int_T\left[\frac{\partial F(\{\alpha\},\{p\})|_{\{p\}}}{\partial\alpha_k}-\{\psi^*\}^T\{R_\Psi(\{\alpha\},\{p\})\}\right]dt \qquad (3-22)$$

where the terms on the right hand side are defined as following.

The individual terms of $\{R_\psi\}$ are given by:

$$r_{\Psi,I} = \int_\Omega N_I \frac{\partial Q_a}{\partial \alpha_k} d\Omega + \int_\Omega \frac{\partial\left(\rho \frac{k_{ij}}{\mu}\right)}{\partial \alpha_k} \rho g_i N_{I,i} d\Omega + \int_{\Gamma_2} N_I \frac{\partial \hat{q}}{\partial \alpha_k} d\Gamma_2 + \sum_{p=1}^{n} \frac{\partial Q_p}{\partial \alpha_k} \delta(x_i - x_p) - \sum_{J=1}^{L} b_{IJ} \frac{\partial \hat{p}_J}{\partial \alpha_k}$$

$$+ \int_\Omega \left[\frac{\partial\left(\rho \frac{k_{ij}}{\mu}\right)}{\partial \alpha_k} \frac{\partial N_I}{\partial x_i} \frac{\partial N_J}{\partial x_j} \right] p_J d\Omega - \int_\Omega \left[\frac{\partial(\phi \rho c)}{\partial \alpha_k} N_I N_J \right] \frac{\partial p_J}{\partial t} d\Omega \qquad (3-23)$$

and the first term on right hand side of equation (3-22) is given by:

$$\frac{\partial F(\{\alpha\},\{p\})}{\partial \alpha_k} = \frac{\partial}{\partial \alpha_k} \int_\Omega f(\{\alpha\},p) d\Omega = \int_\Omega \frac{\partial f(\{\alpha\},p)}{\partial \alpha_k} d\Omega \qquad (3-24)$$

Equation (3-24) represents the direct sensitivity effect which is the first term of right hand side in the marginal sensitivity equation (3-22).

The fist term in equation (3-23) represents the marginal sensitivity of the performance measure to the regional flux Q_a, and other terms represent the marginal sensitivity to the prescribed boundary flux, point flux, prescribed pressure boundaries, hydraulic conductivity and compressibility or porosity respectively.

All terms of equations (3-23) and (3-24) are readily obtainable. It may be pointed out that equation (3-18) is solved backwards in time. The time increments are those specified in the formulation of $[D^{t_i}]$ and $[C^{t_i}]$ in the coefficient matrices of equation (3-18). The primary problem equation (3-1) and the adjoint state equation (3-10) differ in the source term only. Solution procedures should be efficient to take this advantage, since the element-by-element calculation of the derivatives of equation (3-10) can have a procedure similar to that used in the element coefficient matrices of the primary problem. Thus the editing of computer codes can be very efficient for considering this fact.

3.3 Calculation of the Sensitivity Coefficient

This chapter summarizes various methods for calculation of the sensitivity coefficients. The sensitivity coefficient is the partial derivative of state variable, e.g. pressure and piezometric head, with respect to any of the model parameters, e.g. the permeability and it may be expressed as a matrix form as below:

$$[J]_{L\times N}=\begin{pmatrix} \frac{\partial p_1}{\partial k_1} & \frac{\partial p_1}{\partial k_2} & \cdots & \cdots & \frac{\partial p_1}{\partial k_N} \\ \frac{\partial p_2}{\partial k_1} & \frac{\partial p_2}{\partial k_2} & \cdots & \cdots & \frac{\partial p_2}{\partial k_N} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \frac{\partial p_L}{\partial k_1} & \frac{\partial p_L}{\partial k_2} & \cdots & \cdots & \frac{\partial p_L}{\partial k_N} \end{pmatrix} \qquad (4-1)$$

where p is pressure or piezomatric head, k represents parameters such as permeability, L represents the total number of performance measures or observations and N represents the total number of parameters. The sensitivity coefficient matrix plays an important role in solving inverse problems (parameter identification) and optimization problems in which the gradients of objective function in the least square approach and Jacobian matrix in the Gauss-Newton algorithm are represented by sensitivity coefficient matrix.

Methodologies and techniques for calculating sensitivity coefficients have been investigated in the past by several authors. Becker and Yeh (1972) introduced the so-called coefficient method by using the concept of parameter perturbation. Yeh and Yoon (1976, 1981) developed an algorithm for the sensitivity equation method based on the Crank-Nicolson scheme. Jacquard and Jain (1964) developed a method using variational theory to evaluate sensitivity coefficients for parameter identification. Chavent.et al. (1975) extended the method to transient flow, which was referred to as the gradient functional approach in their paper, through solving an adjoint equation. A discussion of the computational aspects of various methods could be found in Dogru and Seinfeld (1981) and Carter (1982) . Sun and Yeh (1985) applied the adjoint state method by the finite element scheme. Li. et al (1987) made a comparative study in the computational accuracy of the various methods.

Since the general forms of the sensitivity state equation and the adjoint state equation have been derived in chapter 2, we now specify the parameters to permeabilities.

3.3.1 Influence coefficient method

This method is based on the concept of plain parameter perturbation. A backward finite difference scheme is used here:

$$\frac{\partial p}{\partial k_l} \cong [p(x_i,t,k_1,k_2,\ldots,k_i+\Delta k_i,\ldots,k_n)$$
$$-(p(x_i,t,k_1,k_2,\ldots,k_i,\ldots,k_n)]/\Delta k_l \qquad (4-2)$$

where $p(x_i,t,k)$ is the solutions of equation (2-18a) with the imposed initial and boundary conditions and Δk_l is the perturbation vector.

Δk_l should be large enough to cause a change in the significant figures of p , but small enough to reduce the truncation error due to the inexact nature of the equation (4-2). If there are L parameters to be identified, the primary equation has to be solved $(N+1)$ times.

3.3.2 Direct equation method

The equation that governs the sensitivity coefficients can be obtained by directly differentiating the flow equation (2-18a) with respect to k_l. Then the state sensitivity equation for calculating the sensitivity coefficient is obtained as below.

$$(\phi\rho c)\frac{\partial \psi}{\partial t} - \frac{\partial}{\partial x_i}\left[\left(\rho\frac{k_{ij}}{\mu}\right)\frac{\partial \psi}{\partial x_j}\right] + D = 0 \qquad (4-3)$$

where $\psi = \partial p/\partial k_l$ and

$$D = -\frac{\partial}{\partial x_i}\left[\frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\partial k_l}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right)\right] \qquad (4-4)$$

The initial conditions and boundary conditions associated with equation (4-3) are:

$$\psi(\Omega,0) = p_0 \qquad \in \Omega, t=0 \qquad (4-5a)$$

$$\psi(\Gamma_1) = 0 \qquad \in \Gamma_1 \qquad (4-5b)$$

$$-\frac{\partial\left(\frac{k_{ij}}{\mu}\right)}{\partial k_l}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right)n_i - \left(\frac{k_{ij}}{\mu}\right)\frac{\partial \psi}{\partial x_j}n_i = 0 \qquad \in \Gamma_2 \qquad (4-5c)$$

where p is the solution of the primary equation (2-18a). Comparing the primary equation (2-18a) and equation (4-3) one can see that the difference between them is only in the source term. So one only requires a modification of the code for the source term of primary equation. The solution of the sensitivity coefficient requires that the primary equation be solved once and the state sensitivity equation be solved N times. So the number of the linear algebraic equation be solved is $(N+1)$ which is the same as that of the influence coefficient method.

3.3.3 Adjoint method

In the adjoint state equation method, if the performance function is considered as below:

$$P = \int_T \int_\Omega p(x_i,t) g(x_i,t) d\Omega dt \qquad (4-6)$$

where $g(x_i,t)$ was defined in equation (2-15). According to equation (2-45) in this case the sensitivity coefficient can be calculated by the equation as below:

$$\frac{\partial P}{\partial k_l} = \int_T \int_{\Omega_i} \left[-\frac{\partial \psi^*}{\partial x_i} \frac{\partial \left(\rho \frac{k_{ij}}{\mu}\right)}{\partial k_l} \left(\frac{\partial p}{\partial x_j} - \rho g_j \right) \right] d\Omega_i dt \qquad (4-7)$$

where Ω_i is the subdomain around the selected nodes. Pressure values p can be obtained from the solution of the primary problem, and the adjoint states ψ^* can be obtained from the solution of the adjoint state equation:

$$(\phi \rho c) \frac{\partial \psi^*}{\partial t} - \frac{\partial}{\partial x_j} \left[\left(\rho \frac{k_{ji}}{\mu} \right) \frac{\partial \psi^*}{\partial x_i} \right] + g(x_i,t) = 0 \qquad (4-8)$$

$$\psi^*(\Omega,\tau) = 0 \qquad \in \Omega, t = \tau \qquad (4-9a)$$

$$\psi^*(\Gamma_1,t) = 0 \qquad \in \Gamma_1 \qquad (4-9b)$$

$$\frac{k_{ji}}{\mu} \frac{\partial \psi^*}{\partial x_i} n_j = 0 \qquad \in \Gamma_2 \qquad (4-9c)$$

The adjoint state equation has the same form as the primary equation. Hence the same numerical scheme can be used to solve p and ψ^*. In this case we need solve the primary equation once and the adjoint state equation l times to generate the sensitivity coefficients. So the number of the linear algebraic equation be solved is $(L+1)$.

A comparison between the mentioned above three methods for calculation on of the sensitivity coefficients shows that the adjoint state method would be advantageous if $N>L$, i.e. the case where the number of perturbed parameters exceeds the number of performance measures. Conversely, if $L>N$, the influence or the direct equation method are preferred.

4 DEMONSTRATIVE SENSITIVITY ANALYSIS OF THE FLOW CONDITIONS AROUND A TUNNEL SYSTEM

In this section, the flow conditions around a tunnel system is investigated by the sensitivity theory. A numerical model developed for sensitivity analysis, in which the theory and methodology of the numerical methods have been developed for solving the primary flow equation, state sensitivity equation, adjoint state equation and sensitivity of performance functions by the Galerkin finite element method, is used to this study. The sensitivity of piezometric head distribution and the sensitivity of the fluxes around the tunnel system due to perturbations of the permeability in various layers are analyzed. The direct and adjoint method both are applied for solving various problems. Various performance measures are considered such as the piezometric heads located in the vicinity of the tunnel system, the Darcy velocity in the vicinity of the tunnel and the total outflux into the tunnel system. The distribution of piezometric heads in the flow domain are also calculated and the mass transport balance in the system is checked.

4.1 The Flow Problem

The flow domain is considered an axi-symmetric vertical cross-section with a lateral of 2 km and depth 1 km. The tunnel is located at depth of about 500 meters below the ground surface. The lateral extent of the tunnel is 600 meters. The bottom and the vertical boundaries are assumed to be a no-flow boundaries (impermeable). On top of the island, the part above the sea level is assumed a prescribed influx boundary which has an average precipitation of $2*10^{-9}$ m/s (63 mm/year). The remaining part below the sea level is considered a hydrostatic pressure boundary. The boundary along the repository tunnel is assumed to be prescribed a pressure boundary which is at atmospheric pressure.

The parameter values used in the calculations are presented in Table 1 below.

Table 1: Parameter values used in the calculations

Symbol	Parameter	Value	Unit
ρ	Fluid density	998	kg/m^3
μ	Dynamic viscosity	0.001	Pas
c^f	Fluid compressibility	4.10^{-10}	1/Pa
c^r	Rock compressibility	0.0	1/Pa
ϕ	Porosity of the rock	0.001	-
g	Gravity	9.81	m/s^2

The considered flow domain is schematically illustrated in vertical cross section in Figure 1. and in three-demensional cross view on Figure 2 below:

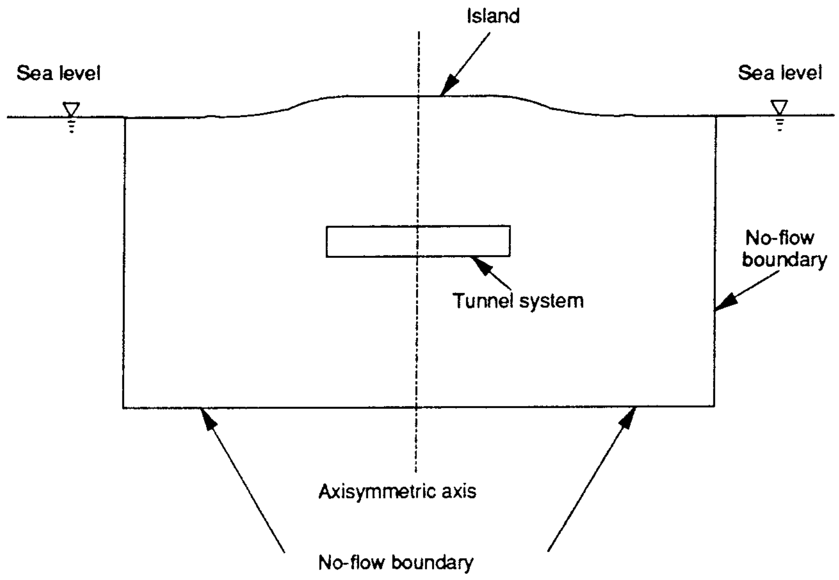


Figure 1: Schematic illustration of the flow domain

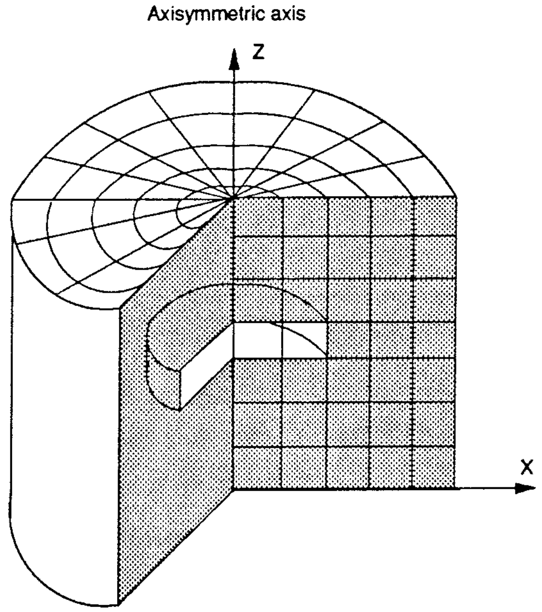


Figure 2: Three dimensional view of the flow domain

Table 2: Distribution of permeabilities in the system

The depth of the layers (m)	The permeabilities (m^2)
0 - 120	$2x10^{-15}$
120 - 500	$5x10^{-16}$
500 - 750	$2x10^{-16}$
750 - 1000	$2x10^{-17}$

The permeability is decreasing with the depth. The flow domain is divided into four layers with different permeability (See Table 2)

The flow domain is discretized in to 120 8-noded quadrilateral elements. The element mesh type is displayed in Figure 3.

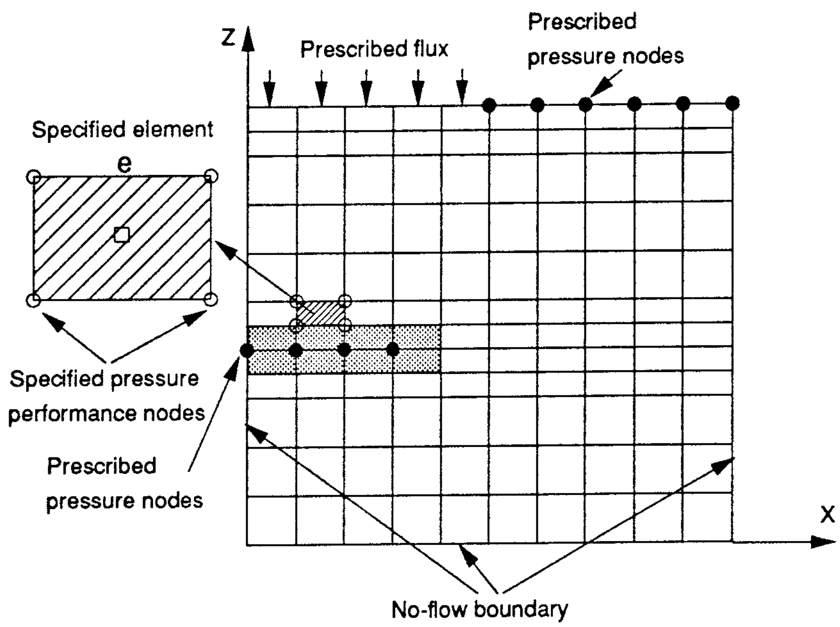


Figure 3: The element mesh of the flow domain

4.1.1 Flow model

The flow considered here is in a three-dimensional inhomogeneous, isotropic, and unconfined aquifer. The governing equation is:

$$\phi\rho(c^f + c^r)p_{,t} - \left[\rho\frac{k_{ij}}{\mu}(p_{,j} - \rho g_j)\right]_{,i} + Q = 0 \qquad (5-1)$$

The boundary and initial conditions are:

$$p(x_i, t) = \hat{p}(x_i, t) \qquad x_i \in \Gamma_1 \qquad (5-2a)$$

$$-\frac{k_{ij}}{\mu}(p_{,j} - \rho g_j)n_i = \hat{q}(x_i, t) \qquad x_i \in \Gamma_2 \qquad (5-2b)$$

$$p(x_i, 0) = p_0(x_i, 0) \qquad x_i \in \Omega, att = 0 \qquad (5-2c)$$

where c is the total compressibility $(c^f + c^r)$, c^f is the compressibility of the fluid, c^r is the compressibility of the rock, $\hat{p}$ is prescribed values of pressure on boundary Γ_1, $\hat{q}$ is prescribed flux normal to boundary Γ_2 (as designated by the components of the unit inward normal), n_i is inward normal vector, $\Gamma = \Gamma_1 + \Gamma_2$ represents the external boundary of the flow domain Ω and p_0 is the initial head over the flow domain Ω. The numerical solutions are worked out using the Galerkin finite element scheme.

4.1.2 Solutions of the flow equation

For convenience to show the flow situation, the solutions are illustrated by the distribution of piezometric head on Figures 4,5. The piezometric head is defined as $h = p/\rho g + z$. The contour lines of piezometric head clearly show that the groundwater flow from the top to the tunnel.

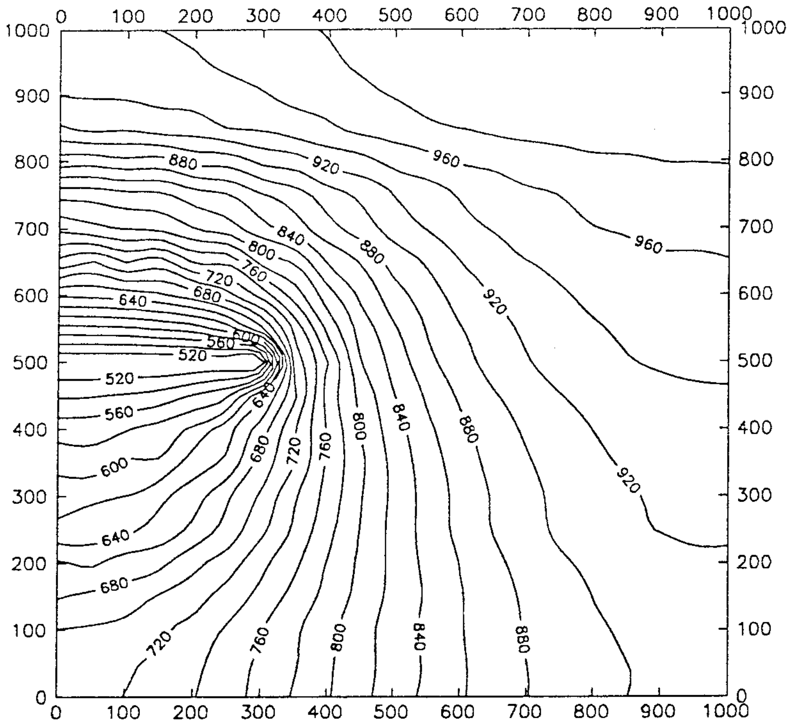


Figure 4: Contour map of the piezometric heads

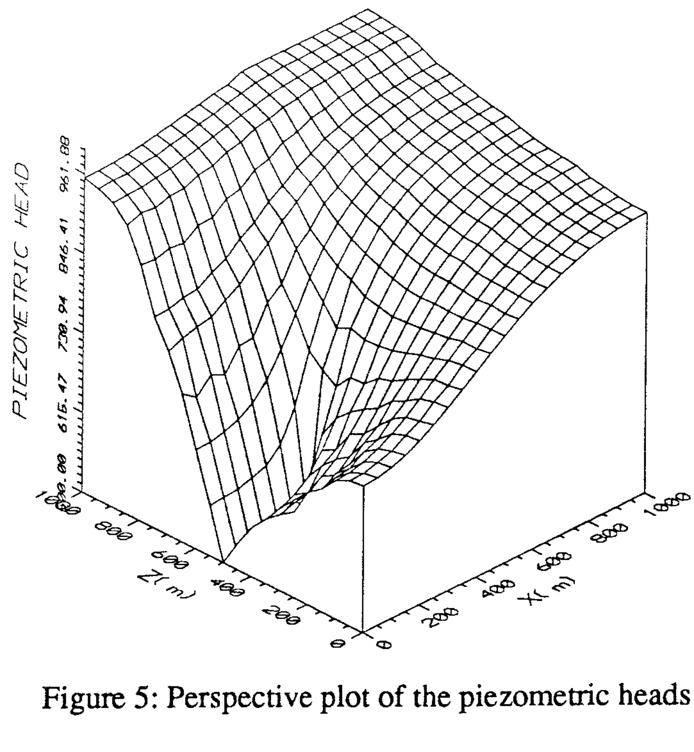


Figure 5: Perspective plot of the piezometric heads

4.1.3 Mass balance calculation

Conservation principle implies that the total influx should equal to the total outflux of the flow domain. Under present case the total flux through the top boundary equal to the outflux into the tunnel. According to Darcy's law :

$$q_i = -\frac{k_{ij}}{\mu}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right) \qquad (5-3)$$

the total influx is obtained by integrating equation (5-3) on the top boundary:

$$Q = \int_{\Gamma} -\frac{k_{ij}}{\mu}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right) n_i d\Gamma \qquad (5-4)$$

In the present case the flow system is assumed to be axi-symmetric. Equation (5-4) can be modified in cylindrical coordinates as below:

$$Q = 2\pi \int_{\Gamma} -\frac{k_{ij}}{\mu}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right) r n_i dr \qquad (5-5)$$

The total outflux is obtained by integrating of equation (5-3) along the boundary of the tunnel. Equation (5-5) can also be used to calculate the flux into the tunnel since the tunnel system is also axi-symmetric. The results are showed in Table 3.

Table 3: The result of mass balance calculation

Total influx (m^3/s)	Total outflux (m^3/s)	Error (%)
0.5177×10^{-2}	0.5371×10^{-2}	2.63 %

4.2 Sensitivity Analysis of the Problem

4.2.1 Calculation of the state sensitivities

The sensitivities of the piezometric head to permeability, *the state sensitivities* or *sensitivity coefficients* are solved by the direct equation method. Since now our problem is the sensitivity of piezometric head on the all nodes in discrete flow domain, so direct equation method is more efficient then the others as mentioned in the former section.

$$(\phi \rho c)\frac{\partial \psi}{\partial t} - \frac{\partial}{\partial x_i}\left[\left(\rho \frac{k_{ij}}{\mu}\right)\frac{\partial \psi}{\partial x_j}\right] + D = 0 \qquad (5-6)$$

where $\psi = \partial p / \partial k_l$ and

$$D = -\frac{\partial}{\partial x_i}\left[\frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\partial k_l}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right)\right] \tag{5-7}$$

The initial conditions and boundary conditions associated with equation (5-6) are:

$$\psi(\Omega, 0) = p_0 \qquad \in \Omega, t = 0 \tag{5-8a}$$

$$\psi(\Gamma_1) = 0 \qquad \in \Gamma_1 \tag{5-8b}$$

$$-\frac{\partial\left(\frac{k_{ij}}{\mu}\right)}{\partial k_l}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right)n_i - \left(\frac{k_{ij}}{\mu}\right)\frac{\partial \psi}{\partial x_j}n_i = 0 \in \Gamma_2 \tag{5-8c}$$

Solution of equation (5-6) gives a direct measure of state sensitivities for each point in the domain.

The distributions of the state sensitivity to permeabilities in four different layers are illustrated in Figures 6-13. As can be observed in the figures the peaks of the state sensitivity are situated mostly in the area around the tunnel in the flow domain.

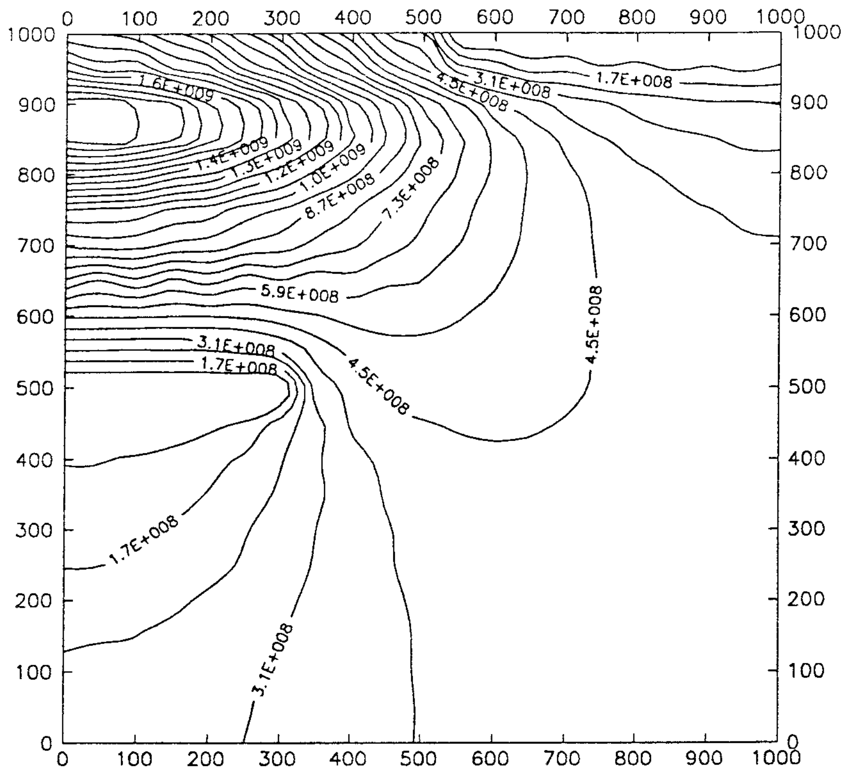


Figure 6: Contour map of state sensitivity for perturbing the first layer

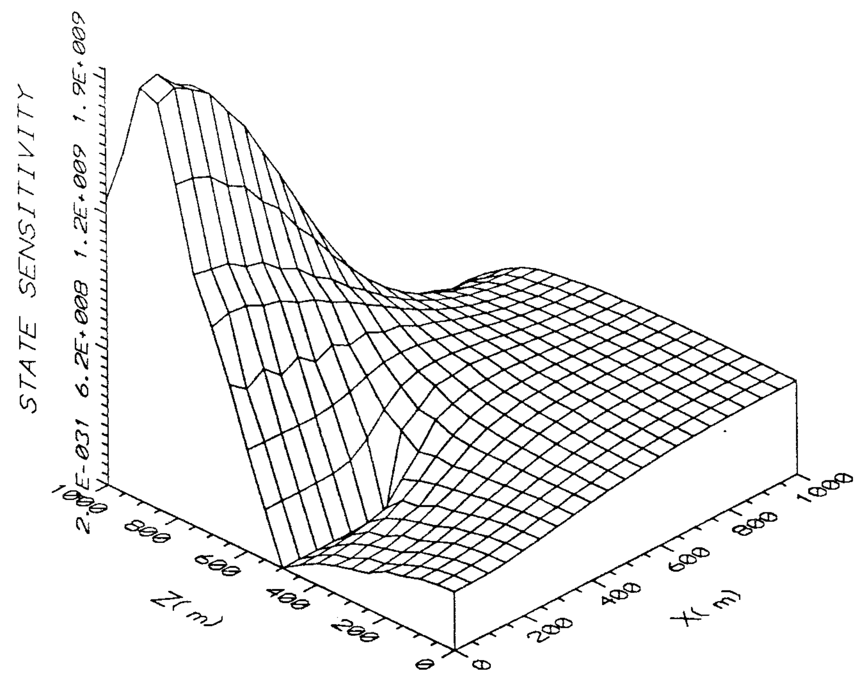


Figure 7: Perspective plot of state sensitivity for perturbing the first layer

$$\frac{\partial h}{\partial T}(x,y,\infty)=\frac{Q}{aT^2}\sum_{m=1}^{\infty}\frac{\sigma(\alpha_m,x,\xi)}{\alpha_m\sinh(\alpha_m a)}\{\cosh[\alpha_m(a-|\eta-y|]$$

$$+\cosh[\alpha_m(a-\eta+y)]\} \qquad (A-16)$$

Results

The solutions of piezometric heads and sensitivity coefficients from the present model show very good agreement with analytical solutions. The comparison of the solutions is shown in Figures A.7 and A.8.

References

Chan, Y.K.,, N. Mullineux, and J.R.Reed, 1976,
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Li, L-S., Sun, N-Z., and Yeh, W.W-G., 1987,
A comparative study of sensitivity coefficient circulation method in groundwater flow, RHO-BW-SA-586 P, January.

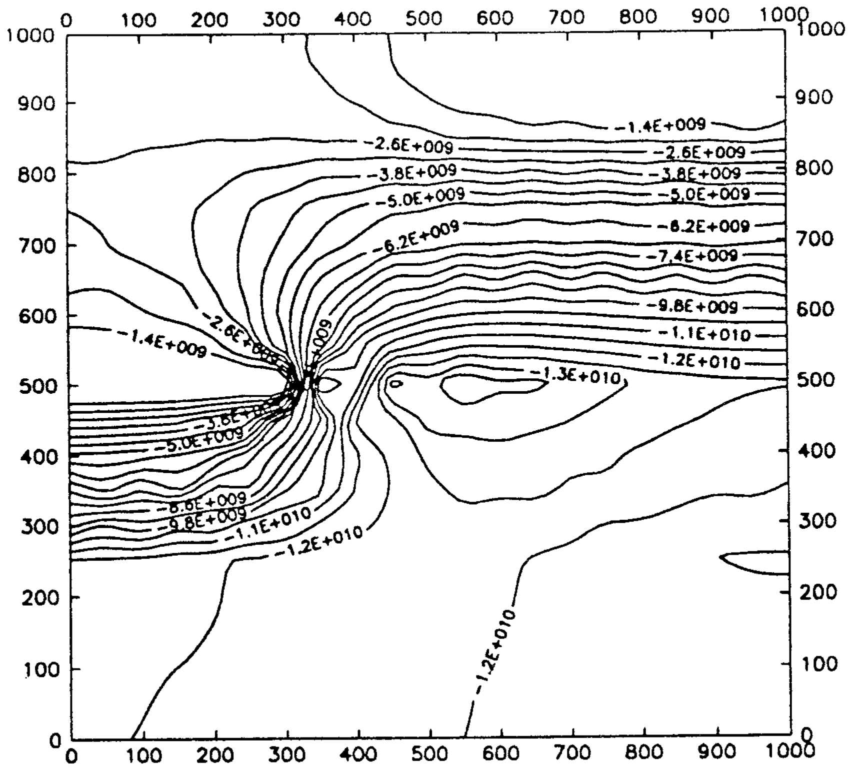

Figure 10: Contour map of state sensitivity for perturbing the third layer

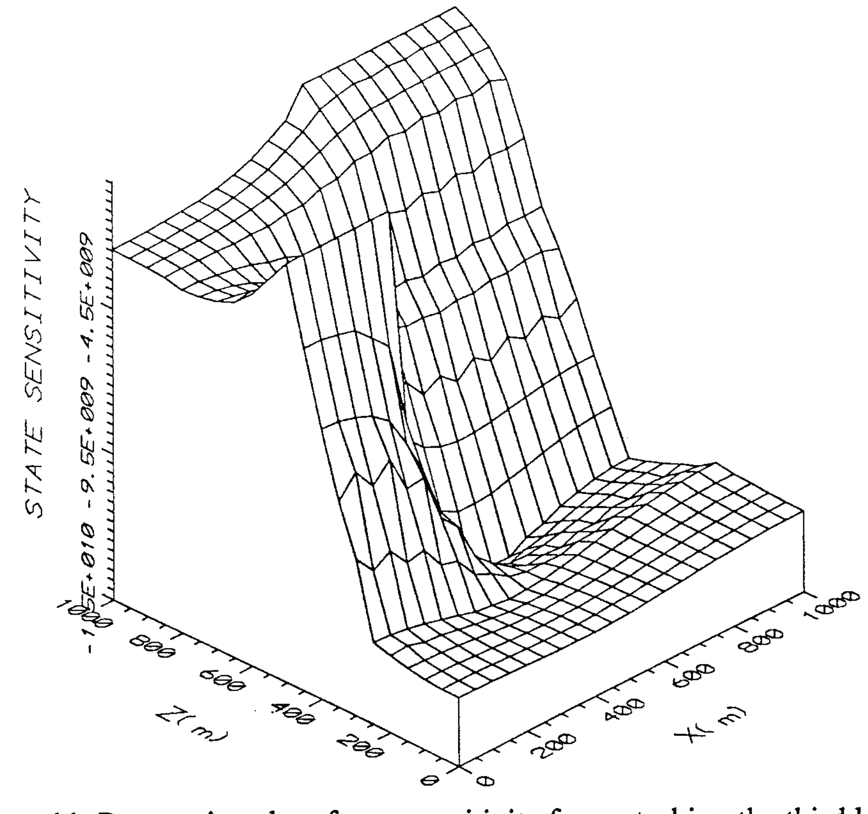

Figure 11: Perspective plot of state sensitivity for perturbing the third layer

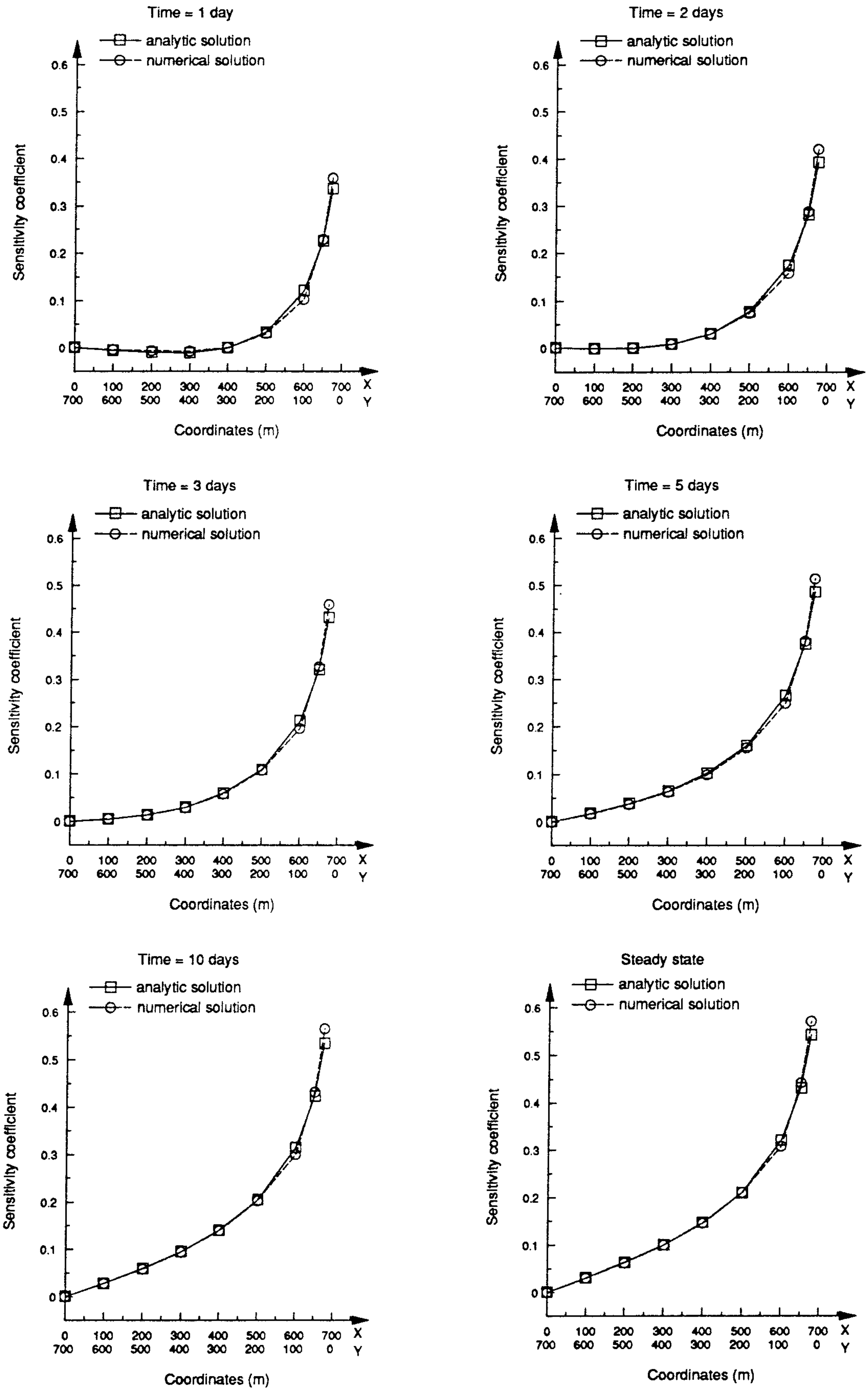

Figure A.8: Comparison of solutions of sensitivity coefficients

4.2.2 Sensitivity of the piezometric head performance function

Here the piezometric heads on the 4 nodes of an element (see Figure 3) located in the vicinity of the tunnel system was considered a performance measure. The sensitivity analysis of this performance measure may give us a measure of the influence of the hydrologic properties on the local piezometric head in the area of interest. The following performance function is considered:

$$P = \int_{\Omega} g(x_i) p(x_i) d\Omega \qquad (5-9)$$

where x_i is a location vector $x_i = \{x_1, x_2, x_3\}$.

Equation (5-10) is used when the performance measure is the pressure, with $g(x_i)$ being an arbitrary weighting function identifying the region of importance.

The performance measure P becomes $P = \{g\}^T \{p\}$ where g are dimensionless weights assigned to the selected node points. Weight $g(x_i) = 1$ at the selected node points and $g(x_i) = 0$ at all other node points. Since in this case the perturbing parameter was specified as permeability in a certain area the marginal sensitivity equation (2-45) can be simplified to the following relationship:

$$\frac{\partial P}{\partial k_l} = \int_{\Omega_i} -\frac{\partial \psi^*}{\partial x_i} \frac{\partial\left(\rho \frac{k_{ij}}{\mu}\right)}{\partial k_l} \left(\frac{\partial p}{\partial x_j} - \rho g_j\right) d\Omega_i \qquad (5-11)$$

where Ω_i denotes the subdomain around the selected nodes and ψ^* is the solution of the adjoint equation which is defined as below:

$$(\phi \rho c)\frac{\partial \psi^*}{\partial t} - \frac{\partial}{\partial x_j}\left[\left(\rho \frac{k_{ji}}{\mu}\right)\frac{\partial \psi^*}{\partial x_i}\right] + \frac{\partial (g(x_i) p(x_i))}{\partial p} = 0 \qquad (5-12)$$

$$\psi^*(\Omega, \tau) = 0 \qquad \in \Omega, t = \tau \qquad (5-13a)$$

$$\psi^*(\Gamma_1, t) = 0 \qquad \in \Gamma_1 \qquad (5-13b)$$

$$\frac{k_{ji}}{\mu}\frac{\partial \psi^*}{\partial x_i} n_j = 0 \qquad \in \Gamma_2 \qquad (5-13c)$$

The third term of the adjoint equation becomes one on the nodes for which sensitivities are sought and becomes zero on all other nodes and the first term becomes zero for the steady state case. Then equation (5-12) becomes:

$$-\frac{\partial}{\partial x_j}\left[\left(\rho \frac{k_{ji}}{\mu}\right)\frac{\partial \psi^*}{\partial x_i}\right] + g(x_i) = 0 \qquad (5-14)$$

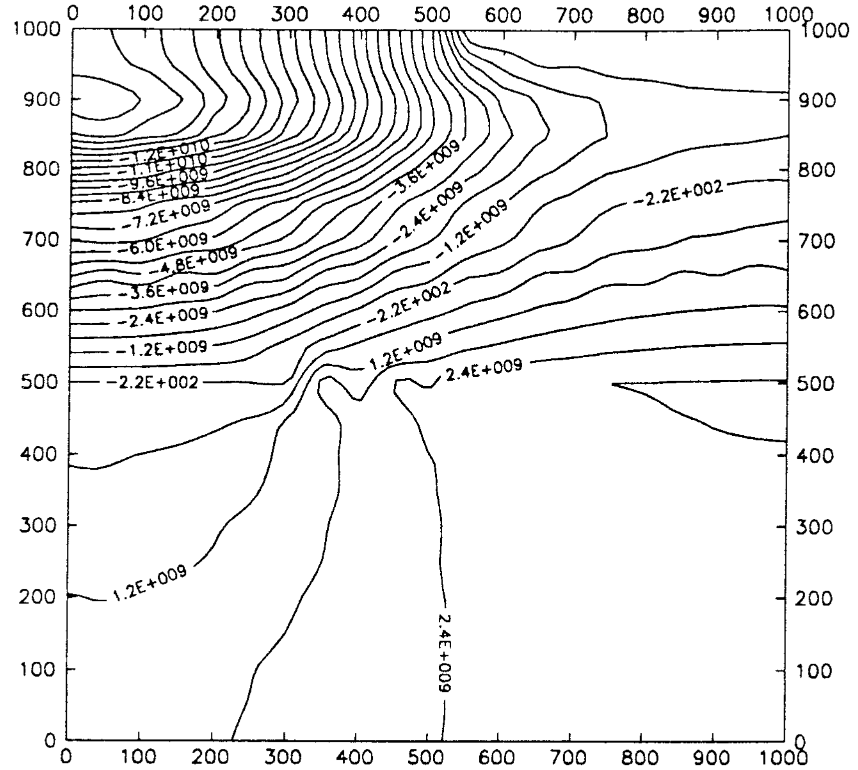

Figure 8: Contour map of state sensitivity for perturbing the second layer

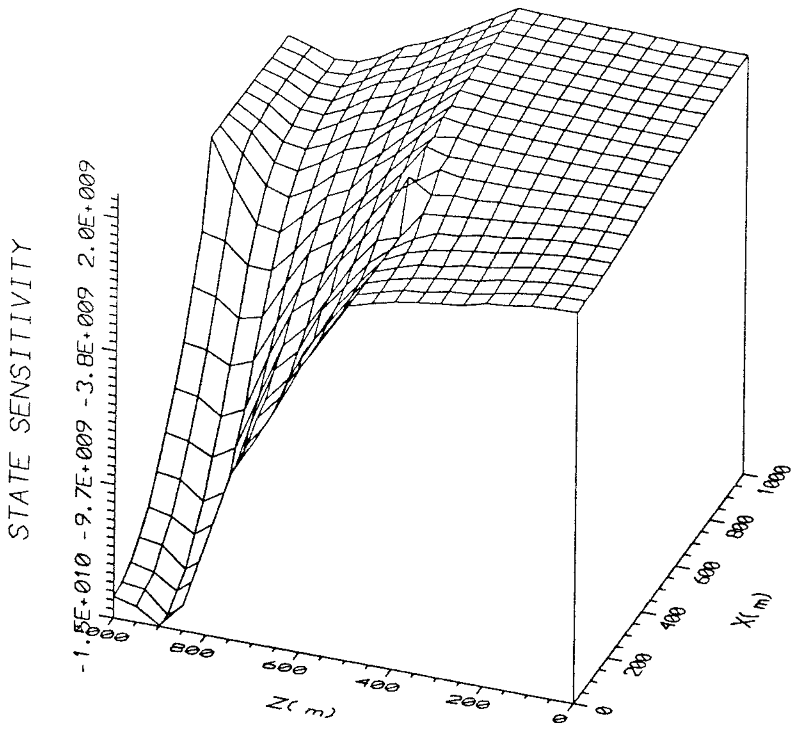

Figure 9: Perspective plot of state sensitivity for perturbing the second layer

$$\frac{\partial Q_{out}}{\partial k_l} = -2\pi \int_\Gamma \left(\frac{1}{\mu}\frac{\partial k_{ij}}{\partial k_l}\left(\frac{\partial p}{\partial x_j} - \rho g_j \right) + \frac{k_{ij}}{\mu}\psi_{,j} \right) r n_i d\Gamma \qquad (5-17)$$

where the pressure p and the state sensitivity ψ are obtained from equations (5-1) and (5-6), respectively.

A dimensionless normalized sensitivity of the flux is defined as:

$$S_k = \frac{dQ}{dk_l}\frac{k_l}{Q} \qquad (5-18)$$

S_k describes the ratio of the relative change of the outflux Q to the relative change of permeability k. The solutions are given in Table 5:

Table 5: The solutions of sensitivities of outflux

Perturbation region (depth m)	Sensitivities of outflux dQ_{out}/dk (Lt^{-1})	Normalized outflux sensitivities S_k(%)
0 - 120	8950	3.3 %
120 - 500	563844	52.5 %
500 - 750	487688	18.2 %
750 - 1000	115841	0.4 %

The results show that the outflux is most sensitive to perturbation of the permeability in the second layer but practically insensitive to perturbations of the permeability in the bottom layer.

4.2.4 Sensitivity of the flux performance function to permeability

The average flux through an element (see Figure 3) located adjacent to the tunnel system was considered a performance measure. The sensitivity analysis of such a performance measure may give us some information about the influence of perturbations of the permeability on the flow velocity in the area near the tunnel. The flux performance function may be defined as below:

$$P = \int_\Omega f(\{\alpha\}, p) d\Omega \qquad (5-19)$$

where

$$f(\{\alpha\}, p) = \sqrt{\sum_{m=1}^{3} q_m^2 \cdot g(x_i)} \qquad (5-20)$$

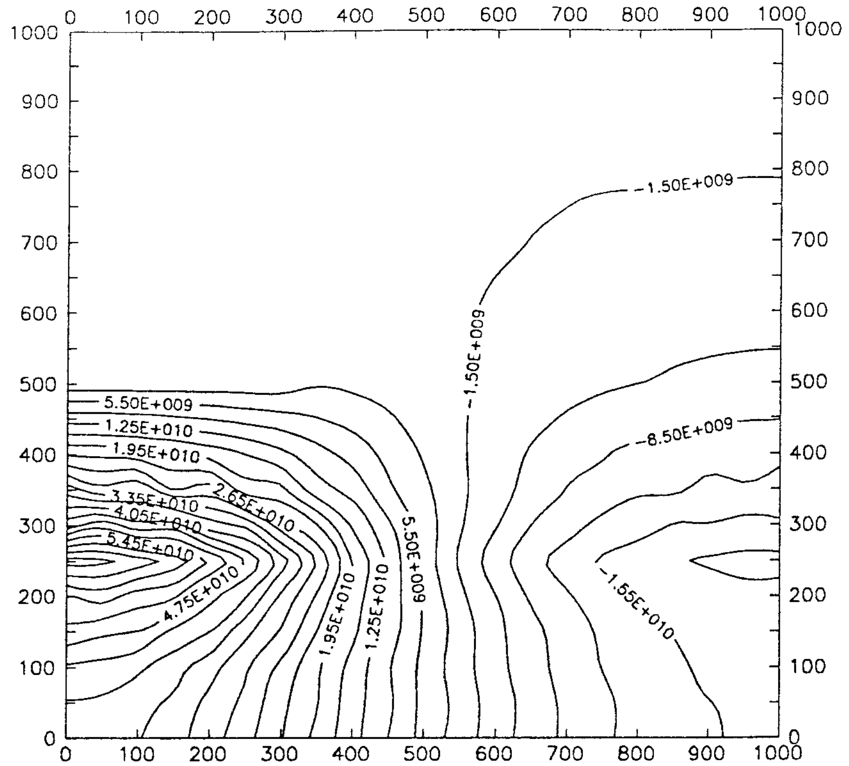

Figure 12: Contour map of state sensitivity for perturbing the fourth layer

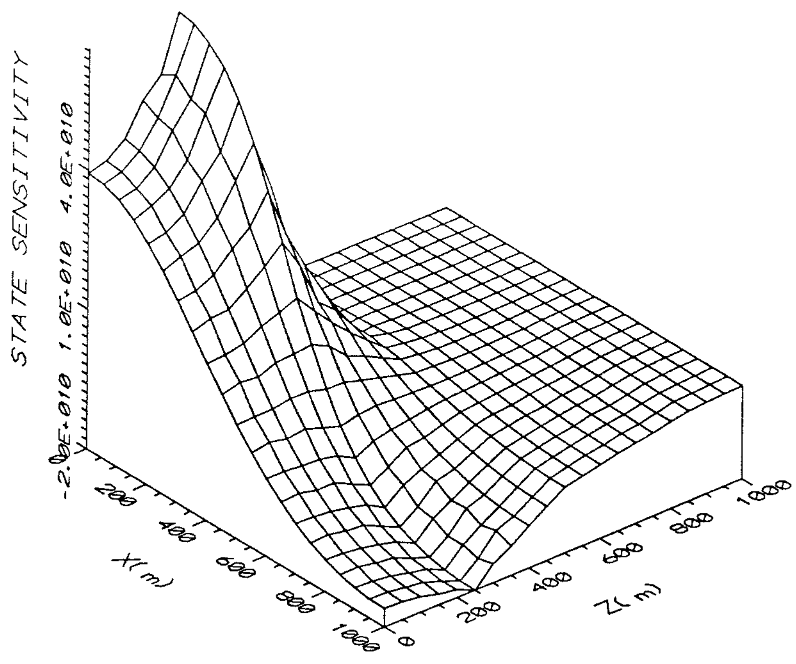

Figure 13: Perspective plot of state sensitivity for perturbing the fourth layer

4.3 Summary of the Calculation Procedure in the Problem Study

The purpose of the present investigation was to analyze the sensitivity of the piezometric head and the sensitivity of the flux for a tunnel system due to perturbations of the permeability. Two different approaches, one which is referred to as the direct method and the other the adjoint sensitivity method, were used. The former method was used to calculate the distribution of the state sensitivities and the flux through the boundary and the latter method was used to calculate various performance functions such as the piezometric head at some specified area, the Darcy velocity.

The numerical method for solving the primary flow equation and the adjoint state equation is based on the Galerkin finite element method. Mass balance calculations were worked out to check the accuracy of the solutions.

The procedure of this study is summarized as follows:

- The piezometric head is obtained by solving the primary flow equation (5-1) together with the initial and boundary conditions (5-2). The mass balance in the system is checked by integrating the flux on the top boundary and along the tunnel boundary.
- The state sensitivities to permeabilities in four different layers are calculated by solving the state sensitivity equations (5-6) to (5-8).
- The sensitivity of the total flux into the tunnel to permeabilities in four different layers is obtained by solving equation (5-17).
- Two performance measures are selected. One is the specified pressure performance function (5-10) and the other is the Darcy velocity performance function (5-20) defined at a selected point in the flow domain.
- The marginal sensitivity of the performance function is calculated by solving equations (5-11) and (5-21). The normalized sensitivity is evaluated by using equations (5-16) and (5-18).

If we consider the piezometric head to be the performance measure instead of the pressure according to the relationship of $h = p/\rho g + z$ then we can obtain the sensitivity of the piezometric head performance function by dividing the results from equation (5-11) by ρg according to the relationship:

$$\frac{\partial h}{\partial k_l} = \frac{1}{\rho g}\frac{\partial p}{\partial k_l} \qquad (5-15)$$

As already mentioned above we selected the piezometric head at 4 nodes in the vicinity of the tunnel (see Figure 3) as a performance measure.

For convenience a dimensionless normalized sensitivity is defined as:

$$S_k = \frac{dP}{dk_l}\frac{k_l}{P} \qquad (5-16)$$

S_k describes the ratio of the relative change of performance measure P to the relative change of permeability k. The solutions of the sensitivity of this performance function are presented in Table 4.

The solutions of the piezometric head performance sensitivity show that the piezometric head is quite sensitive to perturbations of permeability in the area where the selected node is located but practically insensitive to perturbations of the permeability in the bottom area.

Table 4: The solutions of head performance function

Perturbation region (depth m)	Sensitivities of head performance function dP/dk($ML^{-3}t^{-2}$)	Normalized sensitivity of head performance function S_k(%)
0 - 120	-0.752×10^{9}	0.374 %
120 - 500	0.371×10^{10}	0.492 %
500 - 750	0.453×10^{10}	0.241 %
750 - 1000	-0.127×10^{9}	0.0006 %

4.2.3 Sensitivity of the flux into the tunnel system

By direct differentiating equation (5-5) with respect to k_l the equation for calculating the sensitivity of the flux into the tunnel is obtained as below:

methods for calculation of the sensitivity coefficient have been applied: The influence method, the direct equation and the adjoint state method. The sensitivity coefficients considered in the present study were the derivatives of the piezometric head with respect to permeability.

The sensitivity equations and the groundwater flow equations were solved by using the Galerkin finite element method. The primary flow equation was solved by fully implicit backward finite difference approximation of the time derivative. The adjoint state equation was solved by backward finite difference approximation from the final time to the initial time. The primary flow equation, the adjoint state equation and the sensitivity state equation differ only in their source terms implying that only a single decomposition of the matrix system is needed for solving both equations.

A verification exercise of the sensitivity model developed here was performed for a two-dimensional non-steady state flow problem with an analytical solution found in the literature. The sensitivity coefficients for a well test problem were calculated by means of the direct method and compared with the analytical results. Very good agreement between the two solutions was obtained.

The sensitivity model was applied to a three dimensional (axi-symmetric) groundwater flow problem, in which the sensitivity of the piezometric head and the sensitivity of the flux into a tunnel system to perturbations of the permeability was analyzed. In the flow domain the tunnel was represented by a disc located at a depth of 500 m below the ground surface. The radius of the disc was 300 m and the thickness 10 m. From the ground surface down to a depth of 1000 meters, the rock was divided into four layers, each with a different value of the permeability. The tunnel system was located between the two middle layers with the axis of the tunnel disc aligned with the vertical direction.

In the analysis both the direct method and the adjoint method were used. The direct method was used for calculating the sensitivity of the piezometric head distribution. The adjoint method was employed in order to analyze various performance functions such as specified piezometric head responses and flux responses at certain regions of interest. The following performance functions were considered: the total flux into the tunnel, the piezometric head in the vicinity of the tunnel system and the Darcy velocity in the vicinity of the tunnel system.

The results of the calculations for the distribution of the state sensitivity to perturbations of the permeabilities in the four different layers of the rock showed that the peaks of the sensitivity coefficients appear mostly in the area around the tunnel. The solutions of the piezometric head performance sensitivity showed that the piezometric head at the selected nodal point was as expected quite sensitive to perturbations of the permeability in the layer where the point was located, but practically insensitive to perturbations of the permeability in the bottom layer.

which is the magnitude of the Darcy velocity at a selected point which is at the centre of the selected element (see Figure 3).

The marginal sensitivity of this performance function is obtained by the following relationship:

$$\frac{\partial P}{\partial k_l}=\int_{\Omega_i}\left[-\frac{1}{\mu\sqrt{\sum_{m=1}^{3}q_m^2}}q_i\frac{\partial k_{ij}}{\partial k_l}\frac{\partial p}{\partial x_j}-\frac{\partial\psi^*}{\partial x_i}\frac{\partial\left(\rho\frac{k_{ij}}{\mu}\right)}{\partial k_l}\left(\frac{\partial p}{\partial x_i}-\rho g_j\right)\right]d\Omega_i \qquad \forall x_i=x_i' \qquad (5-21)$$

where ψ^* is called the adjoint state sensitivity obtained from equation (5-12). The first term of equation (5-21) is non-zero only when k_l represents the value of k_{ij} within the element e. For this performance function the third term of the adjoint equation (5-12) can be calculated by the following equation:

$$\frac{\partial f}{\partial p_e}=-\frac{1}{\mu\sqrt{\sum_{m=1}^{3}q_m^2}}q_i\frac{\partial\left(k_{ij}\frac{\partial p}{\partial x_j}\right)}{\partial p_e} \qquad \forall \quad e\ on\ the\ element \qquad (5-22)$$

$$\frac{\partial f}{\partial p_e}=0 \qquad \forall \quad e\ not\ on\ the\ element \qquad (5-23)$$

where the pressure p and state sensitivity ψ are obtained from equations (5-1) and (5-6), respectively.

The solutions of this performance measure are given in Table 6.

Table 6: The solutions of velocity performance function

Perturbation region (depth m)	Sensitivities of velocity performance measure dP/dk(Lt^{-1})	Normalized sensitivities of velocity performance measure S_k(%)
0 - 120	-18.14	4.9 %
120 - 500	-1377.4	93.7 %
500 - 750	100.2	0.54 %
750 - 1000	-2.77	0.008 %

The results show that the sensitivity of the velocity performance measure at a selected point (see Figure 3) is most sensitive to perturbations in the area where the point is located and almost insensitive for the perturbing permeability in the bottom layer.

6 NOMENCLATURE

$[A],[B]$	coefficient matrixes in algebraic equations
a_{IJ}, b_{IJ}	individual terms of the coefficient matrix in algebraic equations
c	total compressibility
c^f	compressibility of the fluid
c^r	compressibility of the rock
$f(\{\alpha\},\{p\},t)$	performance function
F	performance function in discrete form
g	acceleration of gravity
$g(x_i,t)$	weighting function
$g(x_i)$	weighting function for steady state
h	piezometric head
k_{ij}	permeability
k_l	perturbed permeability
$[J]$	Jacobian matrix
n	normal inward vector
N	basis function
p	pressure
p_0	pressure at initial state
$\hat{p}$	prescribed pressure
P	performance function in integration form
q	Darcy flux
$\hat{q}$	prescribed Darcy flux
$Q(x_i,t)$	source-sink term
Q_a	regional source
Q_p	point source
Q_{out}, Q_{in}	total outflux or influx
$\{R\}$	vector of source term in algebraic equation
r	individual terms of the source vector
S_k	normalized sensitivity
T	time interval
t	time
t'	specified time
t_i	time step $i = 1,2,\ldots\ldots\tau$
t_τ	final time of a time interval
x_i	space variables
x'_i	specified space variables

5 SUMMARY AND DISCUSSION

Sensitivity analysis is an effective tool for analysing responses of some selected performance measures of a groundwater flow problem to perturbations of various parameters associated with the problem. Performance measures of interest are the piezometric head distribution, piezometric heads in a certain region, flow velocities at certain points, total flux through a certain region or through a boundary. The parameters include prescribed boundary heads or fluxes, permeability or other physical parameters. Sensitivity is usually defined as the derivatives of a specific performance measure with respect to the parameters.

In the present study, a sensitivity analysis of a general set of simulation equations, usually defined by the matrix equation associated with the considered physical problem, is presented in order to facilitate the understanding and application of sensitivity analysis to groundwater flow problems.

Two methods are considered for calculating sensitivities, one is the "direct method" and the other is the "adjoint method". In the direct method the sensitivity equations are obtained by direct differentiation of the primary flow equations, and in the adjoint method variational theory is used to formulate an adjoint sensitivity equation.

The solution of the flow equation, the so-called primary problem, and the adjoint state from the adjoint sensitivity equation then makes it possible to determine all the required derivatives and their related sensitivities.

From the computational point of view, a comparison between the two methods shows that when the number of parameters exceeds the number of performance functions, then the adjoint method is more efficient than the direct method. Conversely, if the number of performance functions exceeds the number of parameters, then the direct method is preferable.

In this study the sensitivity theory was used to establish a specific sensitivity model for three-dimensional transient groundwater flow. The following equations and formulations for the sensitivity model were derived in detail in the continuous form: primary flow equations for evaluating piezometric heads, state sensitivity equation for calculating sensitivity coefficients (i.e. the sensitivity of the piezometric head distribution), adjoint sensitivity equation for solving adjoint function (adjoint sensitivity states), and marginal sensitivity integration for measurement of sensitivity of performance function.

Various performance functions, such as the local piezometric head, the Darcy velocity at certain points in the flow domain, the outflux through a boundary and the sum of the squares of the differences between predicted and measured values, have been developed. The last mentioned performance function is of interest in inverse groundwater flow problems. Three different

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The flux into the tunnel was most sensitive to perturbations of the permeability in the layer next to the top layer, but practically insensitive to perturbations of the permeability in the bottom layer. The sensitivity of the velocity performance at a selected point in the layer next to the top layer was most sensitive to perturbations of the permeability in the layer where the specified point was located and almost insensitive to perturbations of the permeability in the bottom layer.

The application of the sensitivity analysis developed in the present study may be considered a simple uncertainty analysis of a groundwater flow system. The study showed that by selecting performance measures of interest we could obtain useful information about the sensitivities of the performance measures of significance for assessing and appreciating measurements of input system parameters and for investigating the behaviour and structure of a geohydrologic system.

Future research on the subject of sensitivity analysis of groundwater flow should examine the more complex non-linear problems associated with adjoint sensitivity analysis of groundwater flow coupled with mass and heat transport. And further research work is needed to enable the treatment of more complex performance functions than those treated in the present study. For instance, the particle travel time from a prospective radioactive waste repository to the biosphere is a performance measure of interest in the safety of assessment of repository site. And the heads at node points in a regional model, which could be used to describe the boundary of the local model, is another useful performance measure in the study of assessing the importance of regional model parameters. Furthermore, the methods of the estimating system state and the performance measure uncertainty, including quantifying parameters as an input to those methods should be considered.

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$\{\alpha\}$	vector of parameters
x_p	specified space variables with point source located
α_k	perturbation parameter
δ_{ij}	Kroneker delta
$\delta(x - x')$	Dirac function
ρ	density of water
μ	dynamic viscosity
ϕ	porosity
Ω	flow region
Ω_i	specified subdomain
$\Gamma_1 \Gamma_2$	boundary of flow domain
ψ	state sensitivity
ψ_0	state sensitivity at initial state
ψ^*	adjoint state sensitivity
ψ_0^*	adjoint state sensitivity at initial state

Subscripts

i,j	indices used for Cartesian tensor notation, repeated indices indicate summation over these indices (i,j = 1,2,3)
I,J	node indices, repeated indices indicate summation over these indices (I,J = 1,2,...L, where L is the number of nodal points)

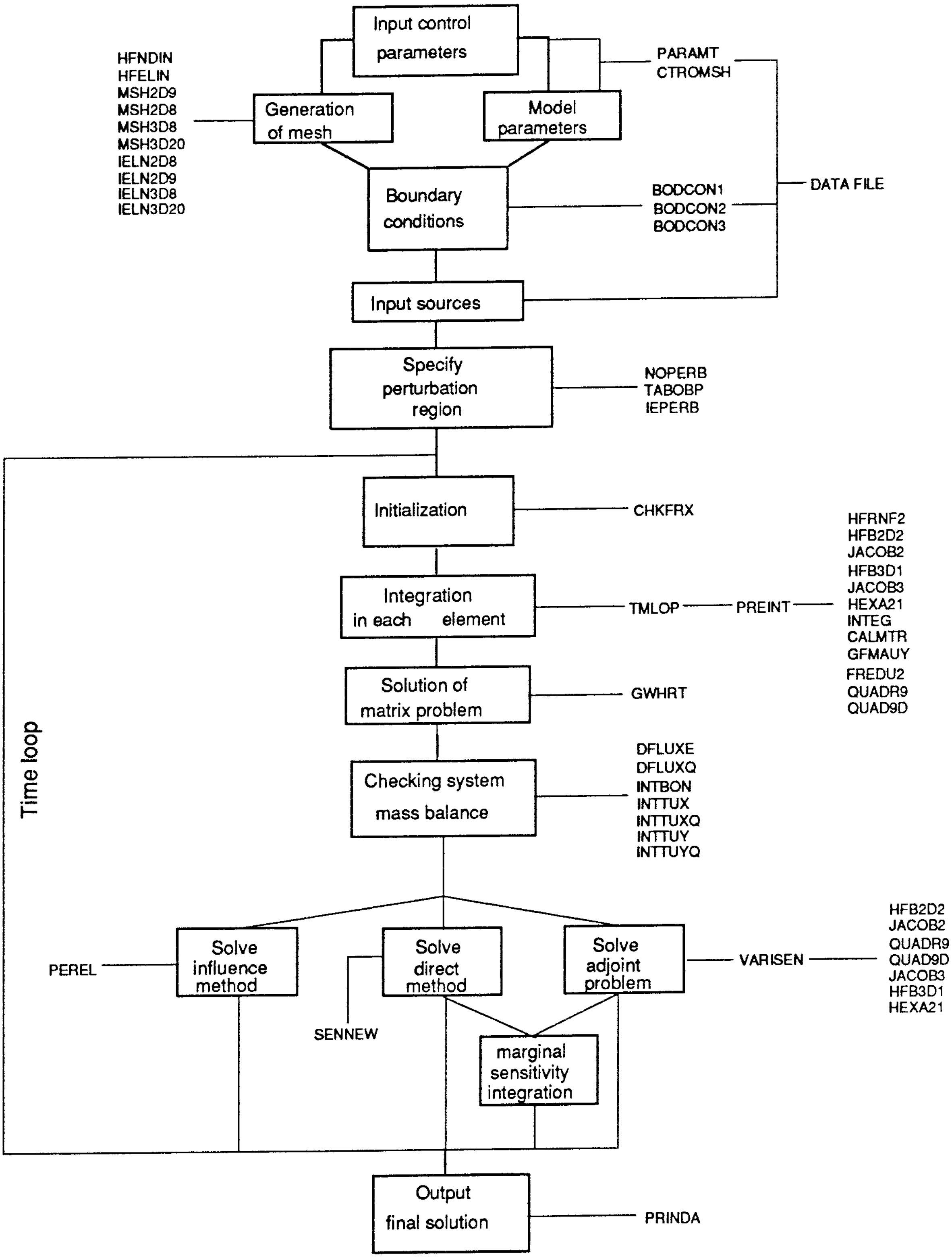

Figure A.1: Program structure chart of GWHRT-S

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--13--The inhomogeneous region IV
XMXPE XMIPE YMXPE YMIPE ZMXPE ZMIPE
1000. 0.0 1000. 880. 0.0 0.0

--14--Water density and viscosity
DENS VISCS
1. 1.

--15--Storativity
STORG
0.0

--16--Initial condition
PINI
0.

--17--Perturbation control parameter & perturbation rate
IHOCPERT PERFAC
1 3.5

--18--The region to be perturbed (Region I)
NPERTRE XMXPE XMIPE YMXPE YMIPE ZMXPE ZMIPE
1 1000. 0.0 250. 0. 0.0 0.0

--19--The nodes to be perturbed
IELPB JOBTAB(1,1) JOBTAB(2,1) JOBTAB(3,1) JOBTAB(4,1)
0 0 0 0 0

--20--The nodes number of point weights
CHEKN JNTAB(1,1) JNTAB(2,1) JNTAB(3,1) JNTAB(4,1)
4 51 53 89 91

--21--The values of point weights
POWET(1) POWET(2) POWET(3) POWET(4)
1 1 1 1

--22--Control options --- ICP2(20) --- (20I3) ----
-Option numbers ---------------------------------------
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
-1 1 2 -2 2 -2 -2 2 -2 -2 -2 2 2 2 2 2 2 2 3 4 5

--23--The parameter of coordinates system IAXSYM = 1 for axi-symmetric
IAXSYM
1

--24--The parameters for controlling performance function
IPERFOR = 1 for head or = 2 for velocity performance function
IPERFOR
1

--25--The element number of velocity performance function
NUVEP
19

--26--The element numbers of the tunnel
NUMTE NUMTT(1,1) (1,2) (1,3) (1,4) (1,5) (1,6) (1,7) (1,8)
8 5 6 17 18 29 30 41 42
NUMTT(2,1) (2,2) (2,3) (2,4) (2,5) (2,6) (2,7) (2,8)
1 1 1 1 1 1 2 2

APPENDIX A

Computational Procedure

A brief description of a computer model GWHRT-S (Thunvik, R and Bao, Y-B 1989) developed for sensitivity analysis of groundwater flow is presented here. Both the direct and the adjoint sensitivity equations may be solved by the model. The numerical techniques of the model are based on the finite element Galerkin method for the spatial discretization and the finite difference method for the time discretization.

The main computational procedures are presented in the following (see Figure A.1):

- Input control variables for selecting the various input parameters, such as boundary conditions, material property parameters, mass sources, perturbation parameters, type of performance functions, location of performance measures, according to the considered problem.
- Generation of element mesh according to particular flow domain of problems to be solved.
- Input of initial conditions.
- Entry time loop. Solution of the flow equation.
- Solution of the sensitivity state equation and adjoint state equation.
- Calculation of the marginal sensitivity. Output final solutions.

Element Types

In the program, 8-nodes and 9-nodes quadrilateral element and 8-nodes and 20-nodes hexahedral element are employed for two dimensional and three dimensional cases respectively. The element types are illustrated in Figure 18.

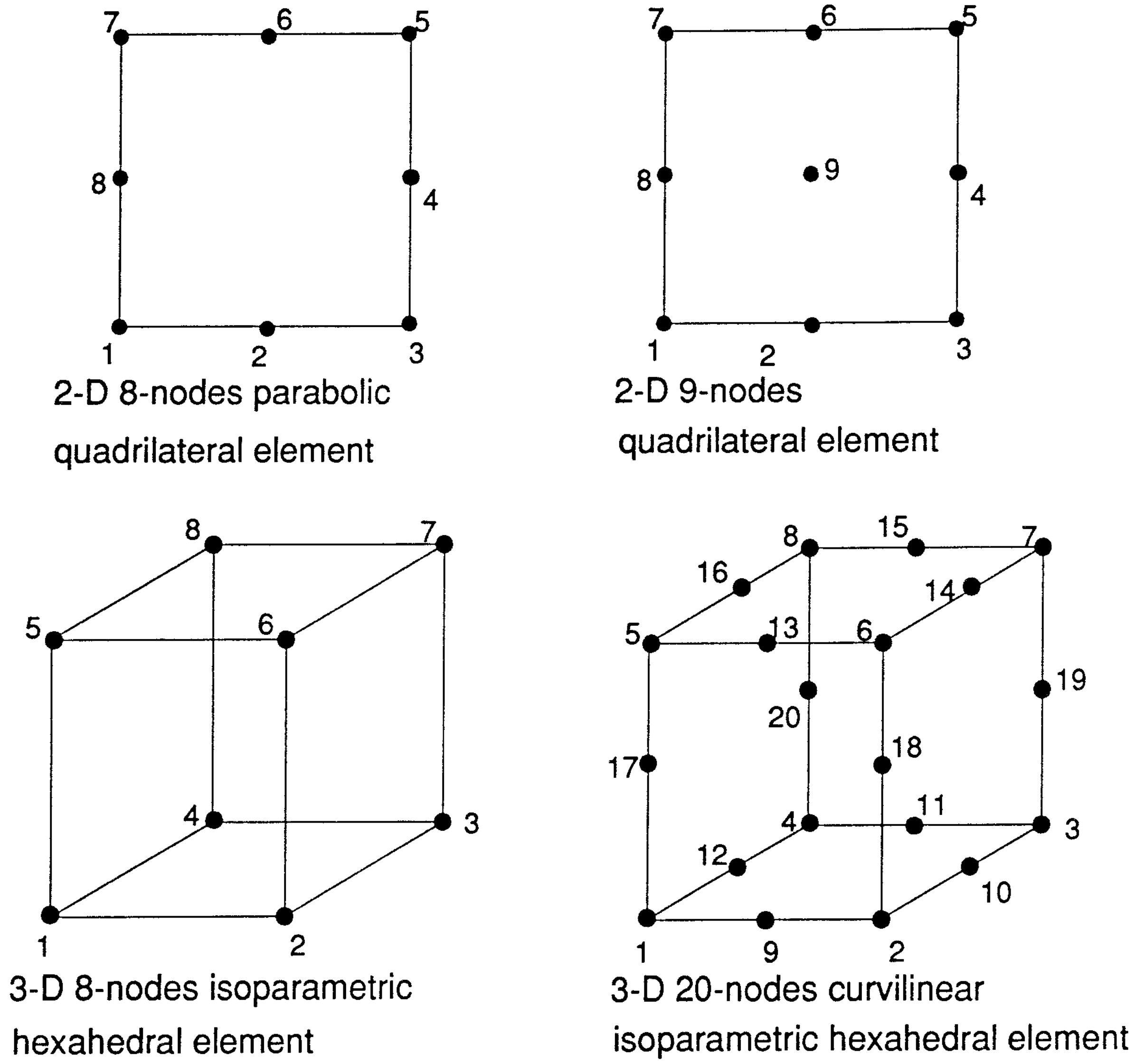

Figure A.2: Element types

Sample of Input Data File

A sample of input data file used in the study of the hypothetical radioactive repository is represented here:

```
**************************************************************

LADAT1.DAT          1989-03-17
 Heading text --------------------------

--01--Time step control parameter
   MXSTEP    DT
   1      10.E28

--02--Parameter to indicate isotropy or anisotropy permeability
   ISOAN  IDEPEND
   0    0

--03--Parameter to indicate relations of components of permeability
   TIMRF(1)   TIMRF(2)    TIMRF(3)
   1        1         0

--04--Parameter to select perturbation component
   ISOPER
   0

--05--The number of inhomogeneous regions
   NUMR
   4

--06--Hydraulic permeability  (Layer I -bottom)
   HCEX(1)  HCEY(1)  HCEZ(1)
   2.E-10    2.E-10  0.

--07--Hydraulic permeability
   HCEX(2)  HCEY(2)  HCEZ(2)
   2.E-9     2.E-9   0.

--08--Hydraulic permeability
   HCEX(3)  HCEY(3)  HCEZ(3)
   5.E-9     5.E-9   0.

--09--Hydraulic permeability  (Layer IV -top)
   HCEX(4)  HCEY(4)  HCEZ(4)
   2.E-8    2.E-8    0.

--10--The inhomogeneous region I
   XMXPE     XMIPE    YMXPE    YMIPE   ZMXPE    ZMIPE
   1000.     0.0      250.     0.      0.0    0.0

--11--The inhomogeneous region II
   XMXPE     XMIPE    YMXPE    YMIPE   ZMXPE    ZMIPE
   1000.     0.0      500.     250.    0.0    0.0

--12--The inhomogeneous region III
   XMXPE     XMIPE    YMXPE    YMIPE   ZMXPE    ZMIPE
   1000.     0.0      880.     500.    0.0    0.0
```

Perturbation Region or Nodes

For analyzing uncertainty of permeability in inhomogeneous flow domain the program can both specify perturbation region or perturbation nodes according to requirement of particular problems. For giving a coordinates of perturbation region, program can search automatically the nodes which are inside the perturbed region. A sample is illustrated in Figure A.5.

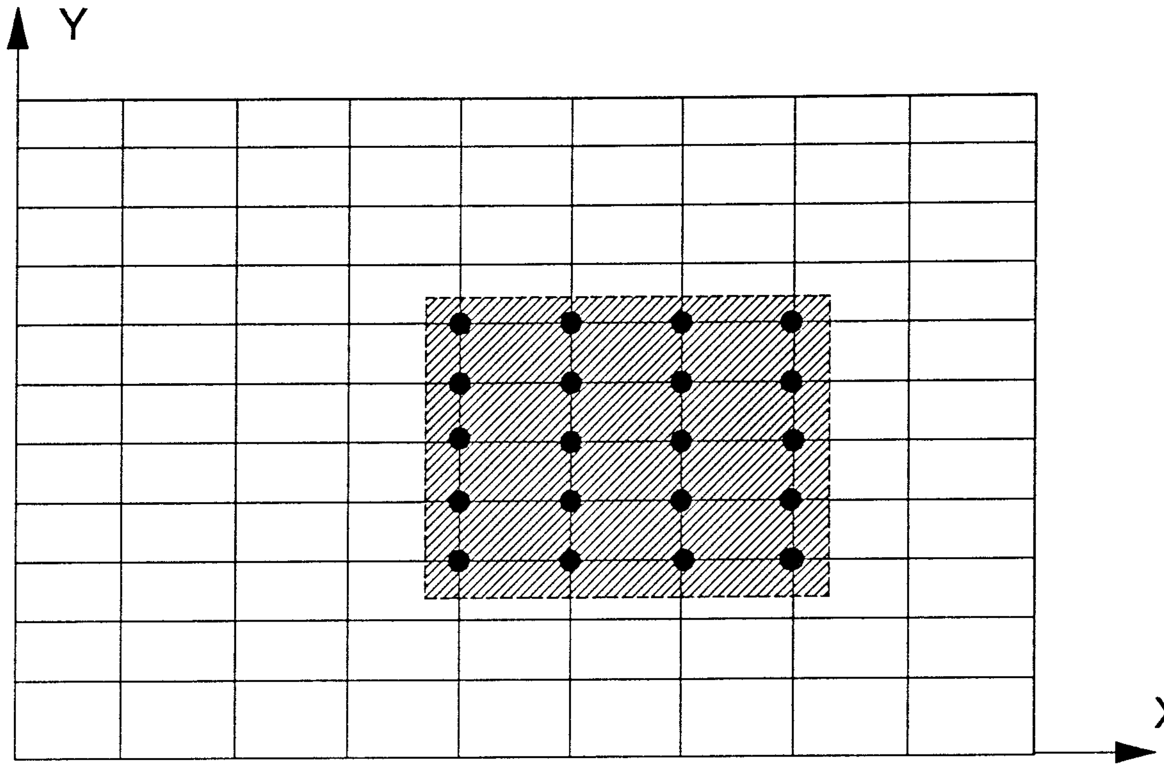

Figure A.5: Sample of specifying perturbed region (20 nodes inside the region)

--27--The element numbers of the top prescribed boundary
NUMBE NUMBB(1) (2) (3) (4) (5) (6) (7) (8) (9) (10)
10 12 24 36 48 60 72 84 96 108 120

--28--The element numbers of the top prescribed flux boundary
NUIEL SUQ
5 2e-9

--29--MESHSP 11 00 Control data for generation of element mesh

--30--Input the size of domain and the numbers of element
TOTLX TOTLY TOTLZ IEX IEY IEZ
1000. 1000 0. 10 12 0.

**-31--The coordinate of layers in X- direction*
XLAY(1) XLAY(2) XLAY(3) XLAY(4) XLAY(5) XLAY(6) XLAY(7) XLAY(8) XLAY(9)
0. 100. 200. 300. 400. 500. 600. 700. 800. 900. 1000.

--32--The coordinate of layers in Y- direction
YLAY(1) YLAY(2) YLAY(3) YLAY(4) YLAY(5) YLAY(6) YLAY(7) YLAY(8) YLAY(9)
0. 100. 250. 400. 450. 500. 525. 550. 600. 725. 880. 975. 1000.

--33--The coordinate of layers in Z- direction
ZLAY(1) ZLAY(2) ZLAY(3) ZLAY(4) ZLAY(5) ZLAY(6) ZLAY(7) ZLAY(8) ZLAY(9)
0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.

***-31--Parameters to control the mesh type*
FACX FACY FACZ
1. 1. 0

--34-- Parameter to control the spatial number and element type
NDIM NNODE
2 8

--35--BODCON 11 00 Control data to set boundary conditions

--36--Boundary condition
PHI1 PHI2
1000. 500.

--37--The number of point sources
NUSOCE
1

--38--The source strength & coordinates of point sources
SOURCEQ XSOCE YSOCE ZSOCE
0.333E-7 0.0 1000. 0.0

****

```
|                                        |-CALMTR
|                                        |-VELOS
|                                        |-DPDPAD
|                                        |-DPDKMS
|                                        |-GFMAUY
|                                        |-SENNEW
|                                        |-FREDU2
|
|------ VARISEN--|-DTIPHQ
|
|------ PRINDA(to printout final solutions)
|
|END
```

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Element Mesh

For generation of the element mesh, either read in the mesh data from developed mesh data file for irregular boundary or element shapes cases or mesh generation subroutine will generate equal or unequal element mesh structure by specified boundary sizes for regular boundary domain. Samples of element mesh are shown in Figure A.3 and Figure A.4.

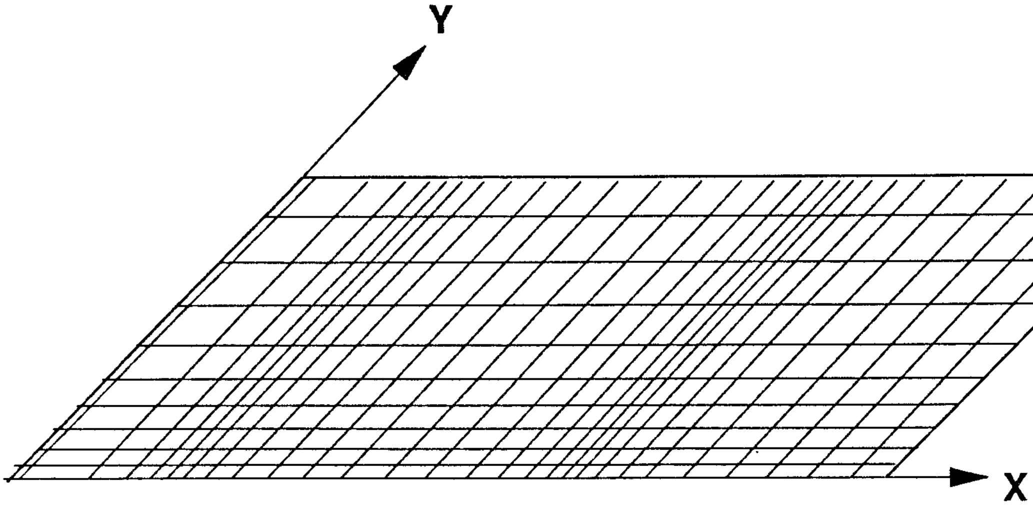

Figure A.3: Sample of 2-D unequal element mesh

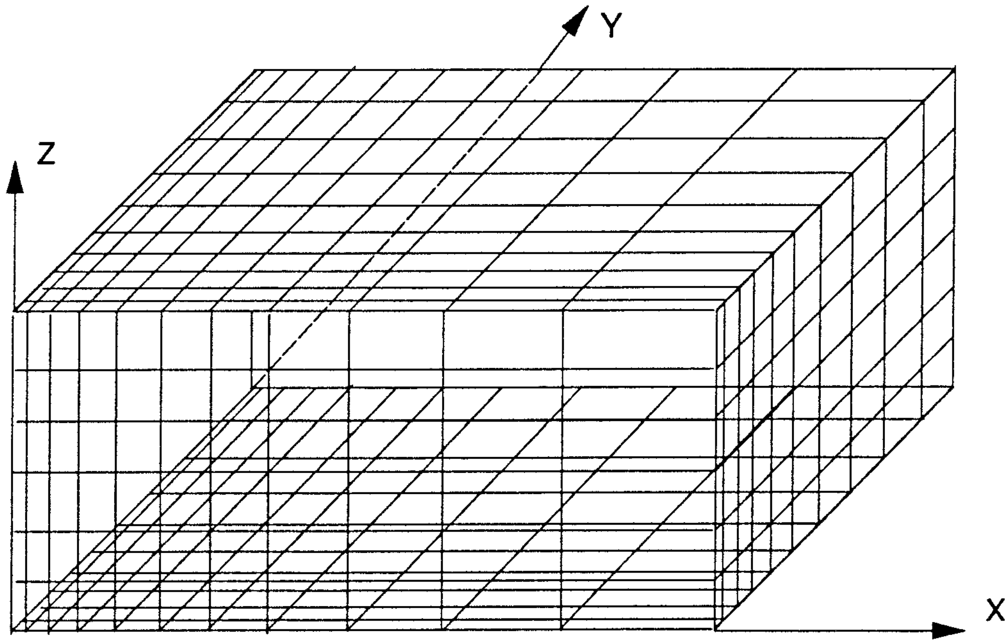

Figure A.4: Sample of 3-D unequal element mesh

The numerical method of solution

The region is divided into 186 quadrilateral 9-noded elements. A pumping well with a pumping rate of 10,000 m^3/d is located at the centre of the aquifer. The governing flow equations are presented as below:

$$\phi\rho(c^f + c^r)p_{,t} - \left[\rho\frac{k_{ij}}{\mu}(p_{,j} - \rho g_j)\right]_{,i} + Q = 0 \qquad (A-1)$$

The boundary and initial conditions are:

$$p(x_i, t) = \hat{p}(x_i, t) \qquad x_i \in \Gamma_1 \qquad (A-2a)$$

$$-\frac{k_{ij}}{\mu}(p_{,j} - \rho g_j)n_i = \hat{q}(x_i, t) \qquad x_i \in \Gamma_2 \qquad (A-2b)$$

$$p(x_i, 0) = p_0(x_i, 0) \qquad x_i \in \Omega \qquad (A-2c)$$

where c is the total compressibility $(c^f + c^r)$, c^f is the compressibility of the fluid, c^r is the compressibility of the rock, $\hat{p}$ is prescribed values of pressure on boundary Γ_1, $\hat{q}$ is prescribed flux normal to boundary Γ_2 (as designated by the components of the unit inward normal), n_i is inward normal vector, $\Gamma = \Gamma_1 + \Gamma_2$ represents the external boundary of the flow domain Ω and p_0 is the initial head over the flow domain Ω.

By using the Galerkin finite element method the algebraic form of equation (A-1) is presented as below:

$$[A]\left\{\frac{dp}{dt}\right\} - [B]\,\{p\} = -\{F\} \qquad (A-3)$$

Using backward finite difference approximation for the time derivative, one obtains:

$$\left[\frac{[A]}{\Delta t} - [B]\right]\{p\}^{n+1} = \frac{1}{\Delta t}[A]\,\{p\}^{n} - \{F\} \qquad (A-4)$$

Where

$$p = \sum_{I=1}^{I} p_I N_I \qquad (A-5)$$

$$[A_{IJ}] = \int\!\!\int_{\Omega}\!\!\int \phi\rho(c^f + c^r)N_I N_J \, d\Omega \qquad (A-6)$$

$$[B_{IJ}] = \int\!\!\int_{\Omega}\!\!\int \rho\frac{k_{ij}}{\mu}N_{J,j}N_{I,i} \, d\Omega \qquad (A-7)$$

Program Organization

```
Main                  Subroutines
----                  -----------
SENMASS --|------ PARAMTA (Read parameters from data files)
          |
          |------ CTROMSH-|--- HFNDIN
          |               |--- HFELIN
          |               |--- MSH2D9
          |               |--- IELN2D9
          |               |--- MSH2D9S
          |               |--- MSH2D8
          |               |--- IELN2D8
          |               |--- MSH2D8S
          |               |--- MSH3D8
          |               |--- IELN3D8
          |               |--- MSH3D8S
          |               |--- MSH3D20
          |               |--- IELN3D20
          |               |--- MSH3D20S
          |               |--- BODCON
          |               |--- BODCON2
          |
          |------ HFIELN
          |
          |------ GAUSSP
          |
          |------ TABCHC
          |
          |------ INHOMG ----|-- NODERB
          |                  |-- TABOBP
          |                  |-- IEPERB
          |
          |------ NOPERB
          |
          |------ TABOBP
          |
          |------ IEPERB
          |
          |------ CHKFRX
          |
          |------ INSUFE
          |
          |------ TMLOP -|-----|-SETCOD
          |                    |-PREINT--|-HFRNF2
          |                              |-INTTUX--|-DFLUXF
          |                              |-INTTUY--|-DFLUXE
          |                              |-INTTUXQ-|-DFLUXQ
          |                              |-INTTUYQ-|-DFLUXQ
          |                              |-HFB2D2
          |                              |-JACOB2
          |                              |-QUADR9
          |                              |-QUADR9A
          |                              |-HFB3D1
          |                              |-JACOB3
          |                              |-HEXA21
          |                              |-INTEG
          |                              |-DRIVT
          |                              |-INTBON
```

$$h(x,y,t) = 100 - s(x,y,\infty) + \frac{20}{a^2T}\sum_{m=1}^{\infty}\frac{\exp(-T\alpha_m^2 t/S)}{\alpha_m^2}\sigma(\alpha_m,x,\xi)$$

$$+\frac{40}{\alpha^2 T}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{\exp(-Tr_{m,n}^2 t/S)}{r_{m,n}^2}\sigma(\alpha_m,x,\xi)C(\beta_n,y,\eta) \qquad (A-13)$$

The steady state solution $s(x,y,\infty)$ is given by

$$s(x,y,\infty) = \frac{Q}{aT}\sum_{m=1}^{\infty}\frac{\sigma(\alpha_m,x,\xi)}{\alpha_m \sinh(\alpha_m a)}\{\cosh[\alpha_m(a - |\eta - y|]$$

$$+\cosh[\alpha_m(a-\eta+y)]\} \qquad (A-14)$$

where

$s =$	drawdown
$S =$	storage coefficient
$T =$	transmissivity
$Q =$	rate of pumping well
$t =$	time
$x, y, =$	Cartesian coordinates
$\xi.\eta =$	coordinates of the pumping well
$a =$	dimension of the aquifer
$m, n =$	integers
$\alpha_m =$	$m\pi/a$
$\beta_n =$	$n\pi/a$
$r_{m,n} =$	$\alpha_m^2 + \beta_n^2$
$\sigma(\alpha_m, x, \xi) =$	$\sin(\alpha_m x)\sin(\alpha_m \xi)$
$C(\beta_n, y, \eta) =$	$\cos(\beta_n y)\cos(\beta_n \eta)$

By taking the derivatives with respect to T in equation (A-13) and equation (A-14), we obtain the analytical expression for sensitivity coefficients as follow:

$$\frac{\partial h}{\partial T}(x,y,t) = -\frac{\partial S}{\partial T}(x,y,\infty)$$

$$+\frac{20}{a^2T}\sum_{m=1}^{\infty}\left\{\left(-\frac{1}{T} - \alpha_m^2 t/S\right)\left[\frac{\exp(-T\alpha_n^2 t/S)}{\alpha_m^2}\sigma(\alpha_m,x,\xi)\right]\right\}$$

$$+\frac{40}{\alpha^2T}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\left\{\left(-\frac{1}{T} - r_{m,n}^2 t/S\right)\left[\frac{\exp(-Tr_{m,n}^2 t/S)}{r_{m,n}^2}\sigma(\alpha_m,x,\xi)C(\beta_n,y,\eta)\right]\right\} \qquad (A-15)$$

For the steady state flow we have

APPENDIX B

A verification exercise of the sensitivity model developed here was performed for a two-dimensional non-steady state flow problem with an analytical solution found in the literature (Chan et al., 1976 and Li et al., 1985). The sensitivity coefficients for a well test problem were calculated by means of the direct method and compared with the analytical results.

The description of the study case

A square, homogeneous, isotropic, and confined aquifer is studied. The flow domain is schematically illustrated in Figure A.6. The dimension of the aquifer is 1,400 m by 1,400 m, and it is surrounded by impervious boundaries AB and CD and constant head boundaries AC and BD, where the piezometric head = 100 m along AC and BD. The transmissivity and storage coefficient of the aquifer are 100 m^2/d and 0.001, respectively. The aquifer is initially in a steady state condition with piezometric head equal to 100 m throughout. For this symmetrical problem a quarter of the region is considered.

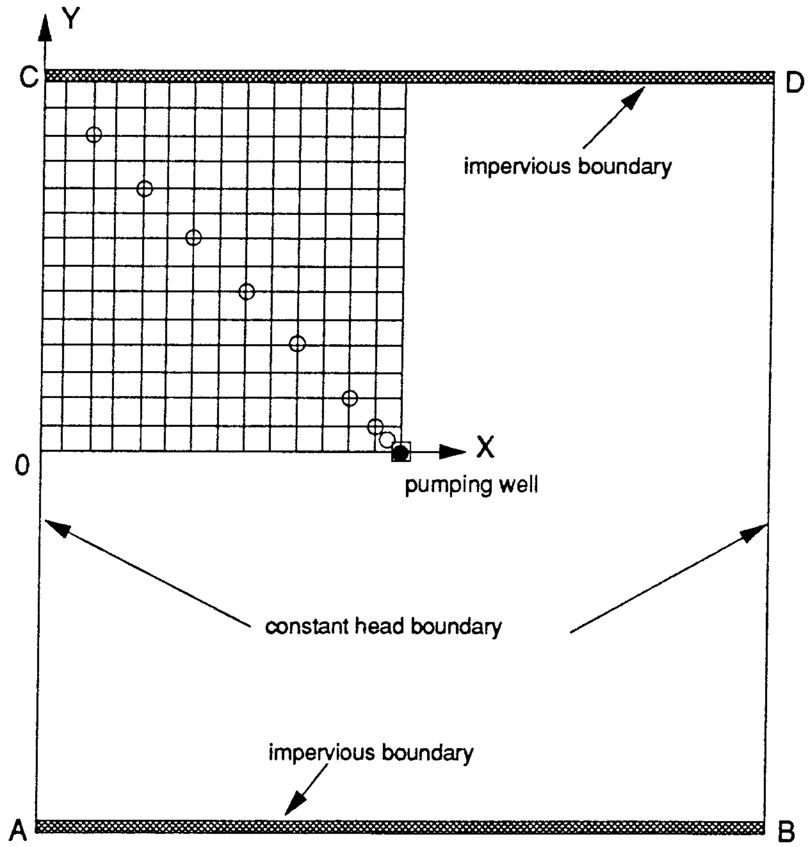

Figure A.6: Aquifer configuration and finite element discretization.

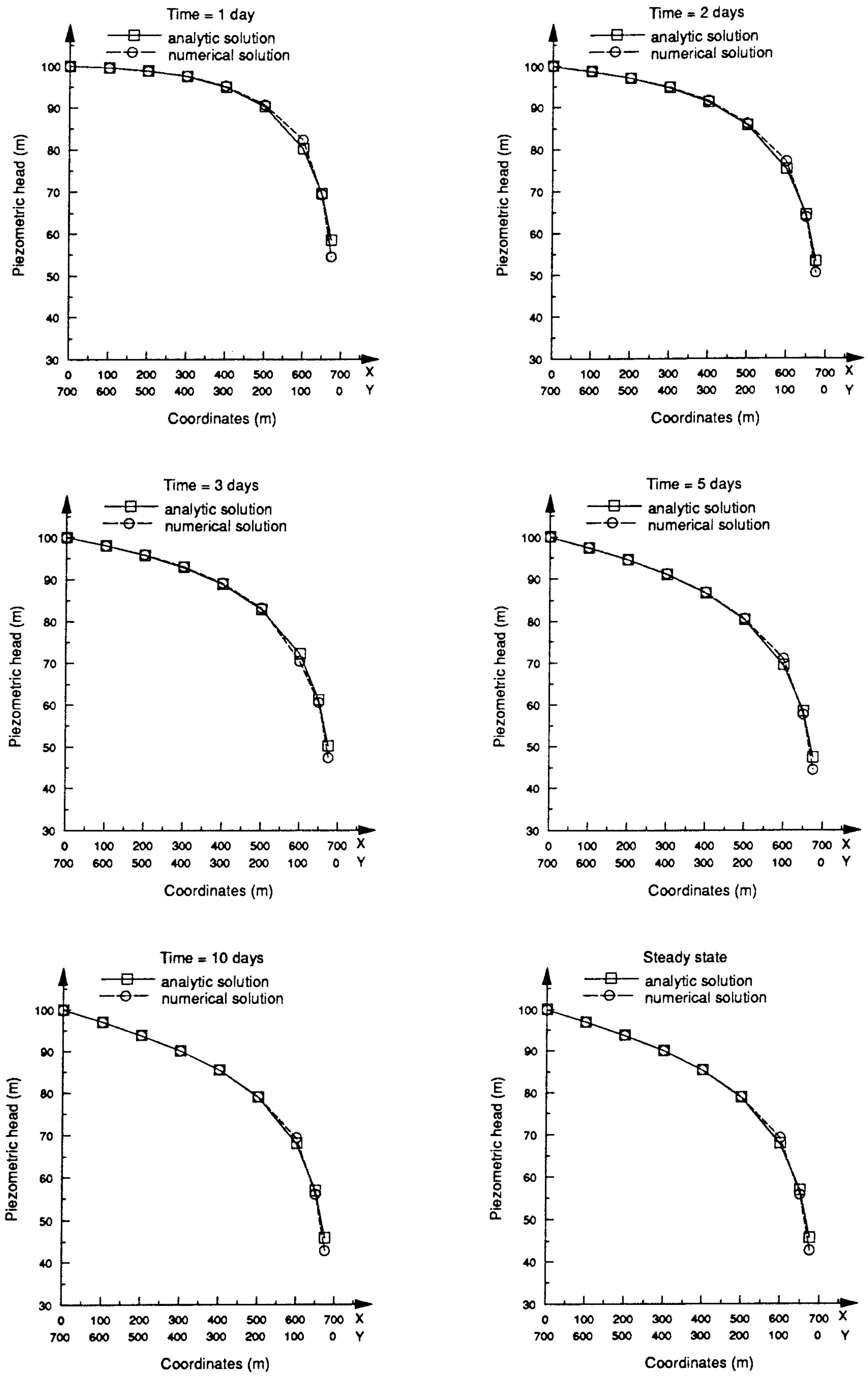

Figure A.7: Comparison of solutions of piezometric heads at transient state

$$\{F_J\} = \iiint_{\Omega} QN_I d\Omega + \iiint_{\Omega} \rho \frac{k_{ij}}{\mu} \rho g_j N_{I,i} d\Omega \qquad (A-8)$$

and n time step level, and N basis function, Δt time step and Q is point sources which is the well in this study.

The equation that governs the sensitivity coefficients can be obtained by directly differentiating equation (A-3) with respect to permeability k. Then one obtains:

$$\frac{\partial[A]}{\partial k}\frac{\partial p}{\partial t} + [A]\frac{\partial(\partial p/\partial k)}{\partial t} - \frac{\partial[B]}{\partial k}p - [B]\frac{\partial p}{\partial k} = -\frac{\partial\{F\}}{\partial k} \qquad (A-9)$$

According to the definitions of equations (A-6) and (A-8), $[A]$ and $\{F\}$ are not functions of k. Then one can obtain the following equation:

$$[A]\left\{\frac{\psi}{dt}\right\} - [B]\,\{\psi\} = \frac{\partial[B]}{\partial k}\{p\} \qquad (A-10)$$

where $\partial p/\partial k = \psi$.

Using backward finite difference approximation for the time derivative, one obtains:

$$\left[\frac{[A]}{\Delta t} - [B]\right]\{\psi\}^{n+1} = \frac{1}{\Delta t}[A]\,\{\psi\}^{n} + \frac{\partial[B]}{\partial k}\{p\}^{n+1} \qquad (A-11)$$

with the boundary and initial conditions:

$$\psi(x_i, 0) = 0 \qquad x_i \in \Omega \qquad (A-12a)$$

$$\psi(x_i, t) = 0 \qquad x_i \in \Gamma_1 \qquad (A-12b)$$

$$-\frac{\partial\left(\frac{k_{ij}}{\mu}\right)}{\partial k_l}\left(\frac{\partial p}{\partial x_j} - \rho g_j\right)n_i - \left(\frac{k_{ij}}{\mu}\right)\frac{\partial \psi}{\partial x_j}n_i = 0 \qquad x_i \in \Gamma_2 \qquad (A-12c)$$

Where p is the solution of equation (A-4). The units of the prescribed values and the variables are transformed to the proper input units according to the present model.

The analytic expression

The analytical expression for the piezometric heads for the case is presented as follow:

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TR 121
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Stockholm, May 1987

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SKB Annual Report 1987
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Stockholm, May 1988

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[1] Starprog AB
[2] SKB AB
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Studsvik Nuclear
January 1990

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Statistical estimation and stochastic simulation using PROPER
Lars Lovius[1], Sven Norman[1], Nils Kjellbert[2]
[1] Starprog AB
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University of Gothenburg, Department of General and Marine Microbiology, Gothenburg
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Department of Nuclear Chemistry, Chalmers University of Technology, Gothenburg
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Studsvik Nuclear
March 1990

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[1] Swedish Nuclear Fuel and waste Management Co (SKB)
[2] Studsvik Nuclear
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H D Schorscher[1], M E Shea[2]
[1] University of Sao Paulo
[2] Battelle, Chicago
December 1990

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I: Osamu Utsumi uranium mine
N Waber[1], H D Schorscher[2], A B MacKenzie[3], T Peters[1]
[1] University of Bern
[2] University of Sao Paulo
[3] Scottish Universities Research & Reactor Centre (SURRC), Glasgow
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M E Shea
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D C Holmes[1], A E Pitty[2], R Noy[1]
[1] British Geological Survey, Keyworth
[2] INTERRA/ECL, Leicestershire, UK
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D K Nordstrom[1], J A T Smellie[2], M Wolf[3]
[1] US Geological Survey, Menlo Park
[2] Conterra AB, Uppsala
[3] Gesellschaft für Strahlen- und Umweltforschung (GSF), Munich
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A B MacKenzie[1], P Linsalata[2], N Miekeley[3], J K Osmond[4], D B Curtis[5]
[1] Scottis Universities Research & Reactor Centre (SURRC), Glasgow
[2] New York Medical Centre
[3] Catholic University of Rio de Janeiro (PUC)
[4] Florida State University
[5] Los Alamos National Laboratory
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N Miekeley[1], O Coutinho de Jesus[1], C-L Porto da Silveira[1], P Linsalata[2], J N Andrews[3], J K Osmond[4]
[1] Catholic University of Rio de Janeiro (PUC)
[2] New York Medical Centre
[3] University of Bath
[4] Florida State University
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N Miekeley[1], O Coutinho de Jesus[1], C-L Porto da Silveira[1], C Degueldre[2]
[1] Catholic University of Rio de Janeiro (PUC)
[2] PSI, Villingen, Switzerland
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J West[1], A Vialta[2], I G McKinley[3]
[1] British Geological Survey, Keyworth
[2] Uranio do Brasil, Poços de Caldas
[3] NAGRA, Baden, Sitzerland
December 1990

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J Bruno[1], J E Cross[2], J Eikenberg[3], I G McKinley[4], D Read[5], A Sandino[1], P Sellin[6]
[1] Royal Institute of Technology (KTH), Stockholm
[2] AERE, Harwell, UK
[3] PSI, Villingen, Switzerland
[4] NAGRA, Baden, Switzerland
[5] Atkins ES, Epsom, UK
[6] Swedish Nuclear and Waste Management Co (SKB), Stockholm
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J Cross[1], A Haworth[1], P C Lichtner[2], A B MacKenzi[3], L Moreno[4], I Neretnieks[4], D K Nordstrom[5], D Read[6], L Romero[4], S M Sharland[1], C J Tweed[1]
[1] AERE, Harwell, UK
[2] University of Bern
[3] Scottish Universities Research & Reactor Centre (SURRC), Glasgow
[4] Royal Institute of Technology (KTH), Stockholm
[5] US Geological Survey, Menlo Park
[6] Atkins ES, Epsom, UK
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L M Cathles[1], M E Shea[2]
[1] University of Cornell, New York
[2] Battelle, Chicago
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D K Nordstrom[1], I Puigdomenech[2], R H McNutt[3]
[1] US Geological Survey, Menlo Park
[2] Studsvik Nuclear, Sweden
[3] McMaster University, Ontario, Canada
December 1990

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N A Chapman[1], I G McKinley[2], M E Shea[3], J A T Smellie[4]
[1] INTERRA/ECL, Leicestershire, UK
[2] NAGRA, Baden, Switzerland
[3] Battelle, Chicago
[4] Conterra AB, Uppsala

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I Puigdomenech[1], I Cass[2], J Bruno[3]
[1] Studsvik AB, Nyköping, Sweden
[2] Department of Chemical Engineering, E.T.S.E.I.B. (U.P.C.), Barcelona, Spain
[3] Department of Inorganic Chemistry, The Royal Institute of Technology, Stockholm, Sweden
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[2] Chalmers University of Technology, Department of Nuclear Chemistry, Gothenburg, Sweden
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[2] Department of Chemistry, Linköping University, Linköping, Sweden
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[2] Chemistry department, University of Zimbabwe, Harare, Zimbabwe
[3] Chemistry Department, State University of New York at Buffalo, Buffalo, NY, USA
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