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Comprehensive Conjunctive-Use Management of Connected Surface Water Groundwater Systems using Stochastic Inputs and Uncertainties

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COMPREHENSIVE CONJUNCTIVE-USE MANAGEMENT

OF

CONNECTED SURFACE WATER GROUNDWATER SYSTEMS

USING

STOCHASTIC INPUTS AND UNCERTAINTIES

by

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ABSTRACT

COMPREHENSIVE CONJUNCTIVE-USE MANAGEMENT OF CONNECTED SURFACE WATER GROUNDWATER SYSTEMS USING STOCHASTIC INPUTS AND UNCERTAINTIES

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A comprehensive conjunctive-use management model is developed. The dynamics of flow and solute transport processes in connected surface water groundwater systems are integrated by a dual programming management model. The governing aquifer flow parameters and streamflows are treated as stochastic random processes. Multiple realizations of the random field are generated and are explicitly incorporated in a non-linear optimization model along with other system, environmental, and management constraints. To facilitate management of large aquifer systems, a linked simulation-optimization approach is used. The simulation program generates the response matrices for flow and transport processes. The management model then determines optimal well discharges and optimal surface water diversion rates. Further, the model determines optimal concentration injection rates for recharge wells and optimal concentration disposal into surface water bodies.

Implicit finite difference method is used in modeling the two-dimensional, unsteady groundwater flow and transport process. Iterative alternating direction implicit method is used in its solution. Leaky aquifer, evapotranspiration, aerial recharge, and induced infiltration can be accounted for. Advection, diffusion, and dispersion of conservative and non-conservative substances are considered in the transport model. In modeling advective component four schemes were investigated. It was found that the quadratic upstream interpolation method is the best.

Implicit finite difference method is used in modeling the one-dimensional, unsteady surface water flow and solute transport processes. The surface water groundwater interaction, stream mass balance, initial and boundary conditions are input to the management model as system constraints.

The individual components of the model developed are tested by comparing the numerical results obtained with analytical solutions and other generic numerical models where available. The model developed is demonstrated for a large aquifer. The considered hypothetical aquifer in model application is based on Yorktown-Eastover aquifer characteristics of Southeastern Virginia Aquifer system.

The comprehensive model developed in this study can be used for field applications of large aquifer systems over a longer management horizon.

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NOMENCLATURE

A	cross sectional flow area
A_s	surface area of the stream (lake) in the cell
b	confined aquifer thickness
C	concentration in the aquifer
C'	solute concentration of the external sources
C'_w	concentration injected through recharge wells
C_w^{max}	maximum concentration injection capacity
C_o	aquifer initial concentration
$C_{d/s}$	concentration at the downstream node
$C_{u/s}$	concentration at the upstream node
$C_{f\,u/s}$	concentration at the far upstream node
C_R	reach concentration
C'_R	effluent concentration disposed into the river
C_R^{max}	maximum concentration disposal capacity in to the river reach
C_w^*	maximum permissible concentration allowed at the pumping wells
C_R^*	maximum permissible concentration in the stream reach
D_x	dispersion coefficient in the X direction
D_{xx}	intermediate dispersive flux term in X direction
D_{yy}	intermediate dispersive flux term in Y direction
D_y	dispersion coefficient in the Y direction
D^*	water demand requirement
D_w^*	portion of the water demand to be met only by groundwater
d_k	reaction coefficient or the decay rate
d_{ks}	first order reaction coefficient for streams
ET^{max}	maximum groundwater evapotranspiration
E []	expected value
h	piezometric head
h_o	aquifer initial piezometric surface
ha	aquifer piezometric head in the river reach
hr	surface water elevation
hr_b	river bottom elevation
it	time step index
jw	pumping well index
js	stream diversion location index
jrw	recharge well index
K_x	hydraulic conductivity in the X direction
K_y	hydraulic conductivity in the Y direction
k	any known point or cell in the aquifer
k	lag (in Eq 3.5.21)

KR	realization index
KT	temporal time step index
m	aquitard thickness
m'	stream bed thickness
N	number of measurements
n	time step index
n	Manning roughness coefficient (in Eq 3.5.6)
NOBS	number of observation wells for initial conditions
NW	number of pumping wells
NWR	number of wells plus river reaches
NRW	number of recharge wells
NRWR	number of potential wells plus river reaches
NSWD	number of surface water diversion points
NDWS	number of waste disposal locations in the stream
NT	total number of simulation or management time steps
NRIVER	number of stream reaches
NDV	total number of decision variables
NTCE	total number of constraints
NLEQ	number of non-linear equality constraints
NLIEQ	number of non-linear inequality constraints
LEQ	number of linear equality constraints
LIEQ	number of linear inequality constraints
P	eigen vectors
P_{zz}	aquitard permeability
P'_{zz}	stream (lake) bed permeability
pde	partial differential equation
Q	Well discharge rate
Q	stream discharge
Q	stationary anisotropic exponential covariance function (in Eq 3.3.2 through Eq 3.3.9, and Eq. A1.2 through A1.26)
Q'	waste discharge rate into the aquifer
$Q_{d/s}$	downstream outflow rate
$Q_{u/s}$	upstream inflow rate
Q_{SWD}	surface water diversion rate from the reach
Q_{SWD}^{max}	surface water diversion capacity
Q_w	pumping well discharge rate
Q_w^{max}	pumping well capacity
Q_{WD}	waste disposal rate into the stream reach
q_{WD}	effluent waste discharge into the stream per unit length
Q_{Yiz}	cross covariance between log parameter at any point i and the measured log parameter
Q_{AR}	areal recharge rate into the aquifer
Q_{ET}	groundwater evapotranspiration rate
Q_{INF}	induced infiltration rate
Q_L	leakage rate
Q_{init}	pumping/recharge rate due to initial conditions

r_k	lag k serial correlation coefficient
r_1	lag-one serial correlation coefficient
RD'	depth below which the evapotranspiration ceases
RH	source bed elevation
RH'	ground surface elevation
RR	areal recharge rate
S	storage of the reach
S_c	storage coefficient of the porous material
S_o	stream bed slope
s	aquifer drawdown due to hydraulic stresses
s^*	maximum permissible drawdown
s_{obs}	known drawdown due to initial conditions
s_β	unit-response coefficient for initial conditions
t	time
t_i	independent normal sampling deviates with mean 0 and variance 1
T1,T3	intermediate flow terms in X direction defined in the advective transport
T2,T4	intermediate flow terms in Y direction defined in the advective transport
T_x	transmissivity in the X direction
T_y	transmissivity in the Y direction
T_w	top width of the stream reach
U	resultant groundwater velocity
Uxx	groundwater velocity in the X direction
Uxy	interpolated groundwater velocity in the X direction
Uyy	groundwater velocity in the Y direction
Uyx	interpolated groundwater velocity in the Y direction
W	volumetric flux per unit area (in Eq 3.2.1)
W	volumetric flux per unit volume (in Eq 3.6.1)
W	weight factor in the weighted difference schemes
W_a,W_c	upstream weight factor on the left and right faces
W_b,W_d	upstream weight factor on the top and bottom faces
$W_{d/s.}$	weight associated with the downstream node
$W_{u/s}$	weight associated with the upstream node
$W_{f\,u/s}$	weight associated with the far upstream node
W_L	wastewater load of the solute injected
W_L^*	waste load demand requirement
WL_{INJ}^*	portion of the waste load to be met only by injection
X	X axis
Y	Y axis
y	stream depth
Y_R	stream depth
Y_R^*	minimum stream flow depth requirement
Y_i	natural logarithm of a hydrogeologic parameter at point X_i
Y_{GC}	Gaussian conditional mean estimate
Y_u	vector of unconditional log parameters
Y_{uGC}	vector of unconditional log parameters based on Gaussian conditional mean estimates

Z	vector of measured log parameters (in section 3.3 and Appendix A1)
Z	distance from far upstream node to the cell wall under consideration
Z	objective function (in Eq 3.10.1, and Eq 3.10.11)
Δt	length of the time step
Δ_f	distance between far upstream and upstream node
Δ_u	distance between upstream and downstream node
Δx_j	grid size of the cell in the X direction
Δy_i	grid size of the cell in the Y direction
α_1, β_1	constant parameters in discharge-area relationship
α_2, β_2	constant parameters in area-depth relationship
β	unit-response function
γ	unit-response concentration function
ϕ	aquifer porosity
λ_i	correlation length scale along dimension i (either X or Y)
μ_y	mean of the random log field
σ^2_y	variance of the random log field
θ	vector of unknown spatial statistical structural parameter of log parameter field

1. INTRODUCTION

All over the world, water resources and its availability is becoming a limiting factor for the growth and development of a region. This is principally due to increase in municipal water consumption, industrial growth, and increase in agricultural activities. More often, it has become a common practice to meet the growing water demands with diverted surface water and pumped groundwater.

The consequence of this increased water demand has resulted in an increase in municipal sewage, industrial wastewater and agricultural wastes. These liquid wastes are disposed either into surface water bodies or through deep injection wells usually after secondary treatment. This process has lead to the pollution of both surface water and groundwater and has sharply increased over the last decade. The maintenance of their water quality within the standard is carried out by regulating the waste load discharged into these receiving bodies. This may be achieved by (i) wastewater treatment and improvement in treatment process, (ii) reuse of wastewater, and (iii) increasing the river self purification capacity, i.e. by increasing water quantity in low flow periods, reservoirs, artificial aeration etc.

In a hydraulically connected surface water and groundwater system, exploitation of any one source may have a direct - even if not an immediate effect, on the other one. For instance, in a connected system, intensive exploitation of groundwater

can result in decreased stream discharge due to induced infiltration, and the quality of water may be affected by its movements from aquifers into surface water and vice-versa. Therefore, the problem of chronic overdraft of an aquifer, diminishing surface water availability and deterioration in quality of both surface water and groundwater in any region are interdependent and are inseparable and have to be treated simultaneously. It is generally recognized that both aspects of water resources - quantity and quality, and both types of water resources - surface water and groundwater - are important and interdependent. Because of this, optimum economic water management requires an integrated approach to the management of both surface water and groundwater. Management procedures should be adequate to avoid any present and future detrimental effects, such as excessive water depletion, deterioration of water quality and land subsidence due to excessive pumping.

Although management plans, goals and interdependency are clearly defined, the single most difficult problem in conjunctive-use management modeling is that of dealing adequately with the effects of model uncertainty in optimal decision making. One important form of model uncertainty stems from the fact that model parameters are uncertain. Therefore, it is necessary to quantify these parameter uncertainties and explicitly incorporate them in the management model, thereby reducing deterministic assumptions. While traditional mathematical description of flow process is deterministic, it is being recognized that because of the nature of streamflows, and natural variability of subsurface flow characteristics, the combined system is inherently stochastic. All these factors affect the water balance in the system and play an essential role in a real system.

Water management plans are only an afterthought, considered when water shortages or other detrimental effects have occurred. In the past years, water resources planning authorities placed development of supplies to meet quantitative demands in their forefront, while increasing attention is now being devoted to quality of water and its management as well. Often water resources planners, development authorities, and agencies face the problem of conjunctive-use operation of the system. The tools made available to them, to manage the entire system are very limited in their scope and applications. To this effect there is a need for a model which addresses all the factors affecting the system as a whole.

The main thrust of this study is in development of a comprehensive conjunctive-use management model for water quality and quantity in connected surface water groundwater systems using stochastic inputs and uncertainties. This is an appreciable step ahead in the state-of-the-art of analyzing regional water resources.

2. LITERATURE REVIEW AND OBJECTIVES OF RESEARCH

Over the last three decades a number of articles have been reported in the literature pertaining to groundwater management models and conjunctive-use management models. Of these, most models are concerned with the development of supplies to meet quantitative demands. Of late, increasing attention is devoted to quality of water and its management. Gorelick (1983) presents extensive literature reviews on the topic, and Yeh (1992) confines literature reviews to groundwater supply management models.

It is only in the last decade the research advances have revolutionized the field of groundwater hydrology to treat heterogeneity and variability of aquifer parameters in a stochastic framework. In this work, stochastic inputs and uncertainties are exclusively included in dealing with aquifer management of water quality and quantity, and has been extended for comprehensive conjunctive-use management of connected surface water and groundwater systems.

In the literature, a numerical method such as finite difference, finite element or method of characteristics is used to frame the management problem, and the solution is attempted by linear programming, mixed integer programming, stochastic linear programming, quadratic programming, nonlinear programming or nonlinear

stochastic programming. In this section, literature reviewed and of primary interest to this research work are grouped into following categories:

a. Stochastic generation of aquifer parameters,

b. Simulation models for flow and transport,

c. Deterministic management models, and

d. Stochastic management models.

2.1 STOCHASTIC GENERATION OF AQUIFER PARAMETERS

The aquifer parameters and heads measured in field, are usually scarce and prone to error. The uncertainty associated with field-measured parameters is an inherent element of subsurface hydrologic simulation. This uncertainty stems from the fact that many aquifer parameters are evaluated indirectly after making few simplifying assumptions. Researchers in early 1970's studied the effects of hydraulic conductivity variations on groundwater flow. Still, the difficulty of obtaining spatial distributions of system parameters was recognized to be a major impediment to wider use of flow and transport models. In later 1970's a new subdivision of hydrogeology, called "Stochastic Hydrogeology" evolved.

Delhomme (1979) pioneered the research in this new area. In his work, he used a geostatistical approach called kriging, which is a linear optimal estimation procedure in characterizing the uncertainty about the transmissivity field of an aquifer. He used conditional simulation for generating different two dimensional realizations that all have the same spatial variability as the true field and are consistent with measured transmissivity values at well locations.

Tang and Pinder (1979) deviated from a geostatistical approach and incorporated the uncertain physical parameters in their engineering analysis of mass transport. In their analysis, they solved the one-dimensional mass transport equation for mean and variance of concentration, given the mean and variance of velocity and dispersion coefficient.

Smith and Freeze (1979) developed a first-order nearest-neighbor stochastic process model to generate a multilateral spatial dependence between hydraulic conductivity values in a block system of one- and two-dimensions. They described the spatial dependence between neighboring values of the random variable by a set of joint probability density functions (pdf).

Notwithstanding recent advances, researchers continued their work on parameter estimation from data and prior information. In all their work, they inferred the stochastic structural parameters (mean, variance, and correlation length scale) characterizing the pdf by some procedure. Kitanidis and Vomvoris (1983) were the first to develop in the field of hydrogeology the widely accepted geostatistically based maximum likelihood estimation (MLE) procedure, using measurements of hydraulic head and permeability. They then used kriging to provide minimum variance and unbiased point estimates of hydrogeologic parameters. In their work, they tested their procedure for a one-dimensional case. Kitanidis and Lane (1985) presented the computational aspects of maximum likelihood parameter estimation using Gauss-Newton method.

Dagan (1985) used the general procedure outlined by Kitanidis and Vomvoris (1983) in seeking the structural parameters characterizing the stochastic field. He used conditional simulation in generating different realizations. Following this, he

solved the inverse problem of groundwater flow using an analytical technique to relate the head and transmissivity variability. In developing his analytical technique few simplifying assumptions were made with respect to the geometry, boundary conditions and inputs.

The evidence in support of assuming log normal distribution and exponential covariance for transmissivity, hydraulic conductivity, and storage coefficient is given in Hoeksema and Kitanidis (1985a). In their work, they analyzed data from 31 regional aquifers to identify the horizontal spatial correlation structure of the aquifer parameters. Their analyses concluded that the logarithms of aquifer parameters pass normality tests. Hoeksema and Kitanidis (1985b) compared Gaussian conditional mean and extended co-kriging methods for their predictive capabilities. They concluded that both applications does provide a good estimate.

Rubin and Dagan (1987a and 1987b) paper is continuation of Dagan (1985) work describing an application of geostatistical approach which used an analytical solution to relate head and transmissivity variability. In their current work they relax few assumptions they had made in their earlier work. Further, they have accounted for the uncertainty associated with the estimation of structural parameters, and incorporated it in predicting conditional mean and covariance of logarithmic parameters. They present an application of their method for Avra Valley aquifer.

2.2 SIMULATION MODELS FOR FLOW AND TRANSPORT

Prickett and Lonnquist (1971) present a finite difference model to simulate groundwater flow. In their work, they use modified iterative alternating direction implicit

(IADI) method to solve the set of resulting finite difference equations. In their report, they include digital computer program listings which can simulate one-, two-, and three-dimensional non-steady flow of groundwater in heterogeneous aquifers under water table, non leaky, leaky artesian conditions. Their program can also handle variable pumpage from wells, natural or artificial recharge rates, surface water groundwater interaction, and groundwater evapotranspiration.

Maddock (1972) derives analytical expressions for the unit response function for the aquifer flow process governed by the linear second order partial differential equation. He refers to these response functions as algebraic technological functions. These unit response functions show aquifer drawdown changes at a set of observation wells induced by a set of pumping wells. Further, in his work, he demonstrates using Green's function that these unit response functions exist even for systems with irregularly shaped boundaries and non homogeneous parameters. He has also demonstrated the use of these functions to explicitly couple groundwater model with a quadratic programming management model to solve the non linear problem of minimizing pumping costs. The constraint set consisted of unit response matrix. Maddock (1974) extended this concept to a combined stream-aquifer system and showed the applicability of the method to conjunctive-use problems.

Morel-Seytoux (1975) derives an integral equation which completely characterizes the interaction between a stream and the alluvial aquifer. To solve pure conjunctive-use of surface water and groundwater problems, the equations are expressed in finite difference form. He gives detailed expressions and numerical procedure to calculate response function coefficients in terms of physical characteristic of the system.

He also gives detailed procedures to handle the aquifer subjected to initial condition in generating unit response functions. He applies his method to a simple conjunctive-use management problem. Linear programming is used in its solution. The model is particularly useful when decisions on pumping rates are to be reviewed on a frequent and regular basis.

Konikow and Bredehoeft (1978) present a model that simulates solute transport in flowing groundwater. Their model couples groundwater flow equations with solute transport equations. They use the method of characteristics to solve the solute transport equation. In their scheme, they use the particle tracking procedure to represent convective transport and a two-step explicit procedure to solve the finite difference equation that describes the dispersion, sources and sinks. In their report, they include computer program listings which can simulate one- or two-dimensional, steady or non steady solute transport. Their model computes changes in concentration over time caused by advection, dispersion, and fluid sources in homogeneous/anisotropic aquifer medium.

Leonard (1979) present a convective modeling procedure using a third order upstream difference scheme which avoids the stability problems of central differencing while remaining free of the inaccuracies of numerical dispersion associated with upstream differencing. His algorithm is based on a conservative control volume formulation. The concentration on the interface is obtained by using a three-point (concentration of the two adjacent nodes to the cell wall together with the concentration of the next upstream node) upstream weighted quadratic interpolation scheme. He gives detailed procedures for solving steady and unsteady one-dimensional advection diffusion equation, and calls it as QUICK and QUICKEST, respectively.

Prickett, Naymik, and Lonnquist (1981) present a "Random-Walk" solute transport model. Their solution is based on the method of characteristics which is also called as particle-in-a-cell technique for convective mechanisms, and a random-walk technique for dispersion effects. The random-walk technique is based on the concept that dispersion in porous medium is a random process. Their report includes detailed procedures and a computer program listing. Their program can handle convection, dispersion, and various types of chemical reactions in one- or two-dimensional, steady/non steady, homogeneous and/or anisotropic groundwater solute transport problems. In short their program can handle a variety of groundwater transport situations.

Leonard (1993) clarifies the misunderstanding about the order of accuracy of his original control volume formulation for a steady one-dimensional QUICK scheme (Leonard, 1979). He concludes that his original scheme is indeed third-order accurate, and his convective-diffusion scheme in a finite-volume formulation is asymptotically twice as accurate as using single point upwind difference scheme (SPUDS) with $(1/6)^{th}$ factor for convection and central difference scheme for diffusion. Further, he concludes both QUICK and SPUDS are formally only second-order accurate because of the dominance of the diffusion terms in the fine grid limit.

2.3 DETERMINISTIC MANAGEMENT MODELS

In this class of models the basic assumption is that all parameters are well defined and known with certainty. To this effect over the last three decades a number of models have been presented in the literature. Here, only those models of primary interest to the proposed research are discussed.

Young and Bredehoeft (1972) presented a linked simulation-optimization approach for conjunctive-use management of groundwater and surface water systems. The system they selected for representation was a 50-mile reach of the South Platte River in northeastern Colorado. Their objective of management was to minimize the impact upon riverflow due to groundwater pumping for irrigation. This would occur if groundwater was used late in the irrigation season and/or wells distant from the river were utilized.

An exhaustive simulation model for flow and chemical quality changes in an irrigated stream-aquifer system was presented by Konikow and Bredehoeft (1974). A finite difference method is used to solve the transient flow of groundwater, while method of characteristic is employed in solving the solute transport portion. The model simulated flow as well as changes in water quality for both, the stream and the aquifer. The model has been applied to the Arkansas river valley of southeastern Colorado.

Morel-Seytoux and Daly (1975) developed a discrete kernel generator for stream-aquifer studies. In their work a finite difference model for aquifer without stream interaction was developed as a first-stage component of a management model of a stream-aquifer system. The finite difference based simulation model generates discrete impulse response coefficients. Each stream reach in the aquifer is viewed as a special well (pumping or injecting). In their paper, a complete description of the discrete kernel generator is provided including basic equations, truncation error propagation, accuracy, and run costs, in solving actual groundwater management problems.

Haimes (1976) presents a joint consideration of the supply and quality of ground and surface water sources in his report on hierarchial modeling for the planning and management of a total regional water resource system. The model is restricted to

linear aquifer systems, where the stream acts as a constant head boundary. However, water quality objectives represent only the conservative and nonconservative pollutant parameters in the stream reaches, and no solute transport in the aquifer is considered.

Optimal conjunctive utilization of groundwater quality and quantity resources of unconfined aquifers under steady state was presented by Willis (1976). The assimilative waste capacity of the aquifer is considered an integral component of the waste treatment system. The objective of the planning model is to optimize the use of the assimilative waste capacity of the aquifer and at the same time preserve the quality of the water supply resources of the groundwater system. The constraints of the mixed integer programming are generated by first spatially discretizing the aquifer and replacing the partial derivatives by finite difference approximations.

Management problem of conjunctive-use of surface water and groundwater via decomposition and multilevel approach was presented by Haimes and Dreizin (1977). This is a comprehensive model dealing with the water quantity aspects. The optimal solution includes a well pumping plan, a recharge plan and surface water use plan.

Marino (1981) presents a two-dimensional, finite element method for simulating the transient movement of water and solute in stream-aquifer systems, the results of which were tested by comparisons with finite difference results for flow portion of the model and with an analytical solution for the solute transport portion. However, the model confines only to the analysis and does not explicitly account for stream diversions to meet quantitative demands.

Illangasekare and Morel-Seytoux (1982) combines the discrete kernel approach for an isolated aquifer with the discrete kernel approach for an isolated stream

to derive a set of influence coefficient tools for a combined stream-aquifer system. They couple the isolated aquifer and stream using a linear relationship for the stream-aquifer interaction. They demonstrate the explicit nature of the relationships between the controllable decision variables and known initial conditions and resulting states of combined stream-aquifer systems in the formulation of management problems.

Optimal dynamic management of groundwater pollutant sources is presented by Gorelick and Remson (1982). In their paper, a linear programming-superposition method is discussed for managing multiple sources of groundwater pollution over time. The method uses any linear solute transport simulation model to generate the unit source-concentration response matrix that is incorporated into the management model. This series of constraints indicate local solute concentration histories that will result from any series of waste injection schedules. Also, flow field variations associated with waste injection are ignored as an approximation. The method is aimed at maximizing groundwater waste disposal while maintaining water quality of local water supplies within desired limits.

On the same lines, the issue of simultaneous utilization of an aquifer for waste disposal and for water supply is presented by Gorelick (1982). In their work, a numerical simulation model of transient solute transport is used to develop a concentration response matrix, which shows concentration histories at points of interest throughout an aquifer resulting from pollutant sources distributed over space and time. When incorporated into a linear programming management model as a constraint, the concentration response matrix enabled maximizing waste disposal activities while protecting groundwater quality.

Peralta et al. (1991) presents a rigorous computational comparison of the two widely accepted techniques of solving groundwater flow problems - the embedding approach and the response matrix approach. They conclude for small systems embedding approach requires less processing time than the response matrix approach. For larger systems response matrix is well suited. However, the embedding approach is preferred even for larger systems if the percentage of pumping cells, and/or if many heads must be constrained or computed within the optimization model.

Dougherty and Marryott (1991) present a simulated annealing approach for optimal groundwater management. Finite difference method is used for the simulation models of flow and solute transport. Simulated annealing is an effective new approach to solve large-scale management problems and its development at this stage is immature, but essentially it is a heuristic and probabilistic optimization method which seeks minima in analogy with the annealing of solids.

Matsukawa et al. (1992) present a conjunctive use planning model for the Mad river basin, California. Nonlinear programming is used to solve the multiobjective planning problem. Their emphasis is on quantity aspects, though water quality is introduced via management constraints.

2.4 STOCHASTIC MANAGEMENT MODELS

Management models that account for spatial variability, uncertainty, reliability and stochasticity are discussed here. In this class of models the basic assumption that all parameters are well defined and known with certainty is relaxed. Only in the last decade, researchers have tried to give a fuller treatment to this class of

models as a result of which rapid development is seen in theoretical research treating flow processes in a probabilistic framework. However, the actual field applications of these methods have been very limited.

Maddock (1974) developed an optimization model for the management of the conjunctive-use of surface water and groundwater, which included uncertainty by way of statistical analysis. The aquifer was modeled with a distributed parameter model. The demands imposed on the sources were modeled as being stochastic. The objective was to minimize the discounted expected energy cost of pumping. This expected cost was derived by including the statistics of the water demand so that the operating decisions are based on the variance and correlation of these demands, as well as on their expected values. The constraints included meeting expected water demand and, on an average, meeting downstream water rights.

Flores et al. (1978) presented a stochastic model for the operation of stream-aquifer systems. The nonlinear optimization problem is solved iteratively using a standard linear programming package. The physical system is represented by a linear reservoir model and a conditional probability approach is used to estimate the effect of parameter variability. It is concluded that stochastic effects are not very important in arriving at an operating policy but are important in determining the expected cost.

A method that has been used to incorporate uncertainty in the optimization model itself is to use chance-constraints, so that certain constraints are not met exactly under all conditions, but instead are only met with a specified level of reliability. Tung (1986) used a response matrix method, with response coefficients generated using the Cooper-Jacob equation in a model to maximize the yield from a confined, homogeneous

and non uniform aquifer without violating head limits specified at various points in the aquifer. The methodology accounted for uncertainty in the aquifer with a single transmissivity and a single storativity by treating them as random variables and formulated the head restrictions as chance-constraints and used first-order analysis and quasilinearization to develop the linear deterministic equivalents of the chance-constraints. Chance-constrained stochastic optimization is used to account for the uncertain nature of these parameters. Spatial variability in model parameters was not considered. The sensitivity analysis at many parameter uncertainty levels indicated that optimal pumping rates were sensitive to aquifer transmissivity and virtually independent of the storativity.

A simulation-regression-management model that explicitly accounts for parameter uncertainty is described by Wagner and Gorelick (1987). The methodology couples three components, (1) groundwater flow and contaminant transport simulation combined with nonlinear least squares regression for simultaneous flow and transport parameter estimation; (2) parameter estimation coupled with response matrix methods to first-order first and second-moment analysis to transfer the information about the effects of parameter uncertainty to the management model and (3) nonlinear chance-constrained stochastic optimization combined with flow and transport simulation for optimal decision making. The methodology was demonstrated for steady state and transient aquifer reclamation design and it was shown that remediation requirements can increase significantly due to parameter uncertainty.

Hantush and Marino (1989) developed a model to maximize the pumping from an aquifer linked to a stream, while maintaining limits on heads in the aquifer and depletion from the stream over time with a specified level of reliability. This model

considered variation in hydraulic conductivity and specified yield due to measurement error, spatial averaging and the "inherent stochastic description" of porous media. It used an analytical approximation to link drawdowns and stream depletion rates due to pumping, and formulated the chance-constraints analytically (using log normal distribution). Sensitivity analysis was also performed to assess the effect of the reliability levels used for the chance-constraints.

Wagner and Gorelick (1989) presented a management approach which accounts for spatial parameter variability and combines Monte Carlo simulation with optimization. This is a nonlinear model based on a response matrix for remediation of a contaminated aquifer. In their model the aquifer piezometric heads are solved for steady state conditions resulting in steady flow velocities as a function of space only. The uncertainty in this problem is due to spatial variability in the hydraulic conductivities. The hydraulic conductivities are assumed to be log normally distributed with the covariance matrix taking an exponential form. Their idea was to generate many possible conductivity realizations and (1) determine minimal pumping sequences which satisfy pollutant concentration constraints under all generated fields or (2) determine minimal pumping sequences for each conductivity realization and characterize optimal pumping by a probability density. Their results indicated that, although this approach is computationally demanding, it leads to reliable management strategies.

A stochastic control method is presented by Georgakakos and Vlatsa (1991). In their work, uncertainty arising from imprecise parameters and boundary conditions are incorporated into the management model. The system equations for a confined aquifer are discretized in space using finite elements and in time using finite

difference, to yield a dynamical system model in state-space form. The stochastic characterization of this system is derived by the small perturbation approach. Management objectives are expressed as a composite performance index which may be used to minimize pumping costs, maintain hydraulic heads and pumping rates or optimally compromise among various system goals. This problem is solved using an open loop feed back control method which exhibits good computational properties.

Wagner et al. (1992) present groundwater quality management under uncertainty. A nonlinear stochastic optimization model for containment of a plume of groundwater contamination through installation and operation of pumping wells is developed. Uncertainty about hydraulic conductivity is explicitly considered. The objective is to minimize the expected total cost of operating the pumping wells plus the recourse cost incurred when containment of the contaminant plume is not achieved. Non symmetric linear quadratic penalty functions are used in the recourse model which affect the frequency and the extent of constraint violations. A finite generation algorithm is used to solve the nonlinear and possibly nonconvex stochastic optimization problem.

2.5 OBJECTIVES OF THE STUDY

Often water resources planners, development authorities and agencies face the problem of conjunctive-use operation of the system. The tools made available to them, to manage the entire system are very limited in their scope and applications. A wealth of the available literature and models deal only with development of surface water or groundwater to meet quantitative demands, of which few of them deal with conjunctive-use management of connected surface water groundwater systems. It is only

in the last decade research emphasis is placed on quality of groundwater. None of the models reported handles management of water quality in connected surface water groundwater systems. Recent research advances in the field of groundwater hydrology to treat heterogeneity and variability of aquifer parameters in a stochastic framework has not paved its way into management models. Also, linked simulation-optimization procedures, and stochastic management models are still in the development stage and field applications of these models are very limited.

The main thrust of this research work lies in the development of a comprehensive conjunctive-use management model in connected surface water groundwater systems using stochastic inputs and uncertainties. The main objectives of this study are:

a. Development of a linked simulation-optimization management model for water quality and quantity in a hydraulically connected surface water groundwater system,

b. The flow and contaminant transport process is considered to be transient process and the combined system is used for water supply and waste disposal of conservative and non-conservative substances,

c. Spatial variability of the aquifer parameters are considered explicitly by generating spatial random stochastic fields,

d. The uncertainties associated with spatial random stochastic fields is minimized by simultaneously introducing multiple realizations of the random field into management model, and

e. Streamflow is considered as stochastic flow process.

3. METHODOLOGY

The overall methodology used in this research work on Comprehensive Conjunctive-Use Management is discussed in this section. Various components of the system are integrated to achieve the stated objective. The mathematical framework for these components are detailed individually.

3.1 CONTROL-VOLUME APPROACH

Throughout this research work the control-volume approach is utilized for the solution of groundwater flow component, surface water flow component, groundwater solute transport component, and surface water solute transport component. In the control-volume method used here, the physical law of mass conservation is applied to a control volume in the neighborhood of a block centered finite difference grid point. This method is considered to be the most practical approach. The single most advantage of this method is that it quickly leads to expressions that can be easily modeled and it has proved to be more accurate near boundaries, as the method keeps the discrete nature of the solution method in view at all times.

3.2 GROUNDWATER FLOW COMPONENT

The groundwater flow component is based on the hydraulic equation describing two-dimensional aquifer type flow. However, the aquifer characteristics are treated in a stochastic manner.

3.2.1 Hydraulic Equations

The two-dimensional, horizontal flow equation under non-equilibrium conditions in a heterogeneous and anisotropic aquifer is described by the pde

$$\frac{\partial}{\partial x}\left(K_x\, b\, \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\, b\, \frac{\partial h}{\partial y}\right) \pm W = S_c \frac{\partial h}{\partial t} \qquad (3.2.1)$$

where, K_x and K_y = hydraulic conductivities in X and Y directions, respectively, h = piezometric head, b= thickness of the aquifer, W = volumetric flux per unit area and represent sources and/or sinks of water, S_c = storage coefficient of the aquifer, and t = time.

In order to solve the above equation (Eq. 3.2.1), appropriate initial condition and boundary conditions in X and Y directions are needed. The initial piezometric surface serves as the initial condition. The boundary conditions could be either Dirichlet (of prescribed head) type or Neumann (of prescribed flux) type.

The block centered finite difference formulation of this equation follows from the application of the continuity equation: sum of all flows into and out of a cell (i,j) that has sides Δx_j and Δy_i must equal rate of change of volume of water per unit horizontal area of the aquifer element. Using a fully implicit approach, the finite difference equation is obtained as

$$\left(\frac{Tx_{i,j-1}+Tx_{i,j}}{2}\right)\left(h^{n+1}_{i,j-1}-h^{n+1}_{i,j}\right)\frac{\Delta y_i}{\left(\frac{\Delta x_{j-1}+\Delta x_j}{2}\right)} +$$

$$\left(\frac{Tx_{i,j+1}+Tx_{i,j}}{2}\right)\left(h^{n+1}_{i,j+1}-h^{n+1}_{i,j}\right)\frac{\Delta y_i}{\left(\frac{\Delta x_{j+1}+\Delta x_j}{2}\right)} +$$

$$\left(\frac{Ty_{i-1,j}+Ty_{i,j}}{2}\right)\left(h^{n+1}_{i-1,j}-h^{n+1}_{i,j}\right)\frac{\Delta x_j}{\left(\frac{\Delta y_{i-1}+\Delta y_i}{2}\right)} + \qquad (3.2.2)$$

$$\left(\frac{Ty_{i+1,j}+Ty_{i,j}}{2}\right)\left(h^{n+1}_{i+1,j}-h^{n+1}_{i,j}\right)\frac{\Delta x_j}{\left(\frac{\Delta y_{i+1}+\Delta y_i}{2}\right)} \pm$$

$$Q^n_{i,j} = S_{c_{i,j}}\Delta x_j \Delta y_i \left(\frac{h^{n+1}_{i,j} - h^n_{i,j}}{\Delta t}\right)$$

where, $Tx_{i,j} = b_{i,j} Kx_{i,j}$, $Ty_{i,j} = b_{i,j} Ky_{i,j}$, $Q_{i,j}$ = flow rate of sources and/or sinks, and n is the time step. Fig. 3.1 shows the cell numbering notation used in the block centered finite difference grid formulation.

As can be seen from the above equation, the flow model has only one state variable: the hydraulic head, h(x,y,t). Solution to this flow model provides predictions of head as a function of space and time. The solution method used here is based on the Iterative Alternating Direction Implicit (IADI) method. This technique is well documented in the generic finite difference model (PLASM) developed by Prickett and Lonnquist (1971).

Iterative Alternating Direction Implicit (IADI) method used here can be summarized as follows. In the first iterative cycle, a set of implicit linear equations in a tridiagonal form is generated for each individual column of nodes. Column by column, the equations are generated and solved. Once all the columns are solved, a set of implicit

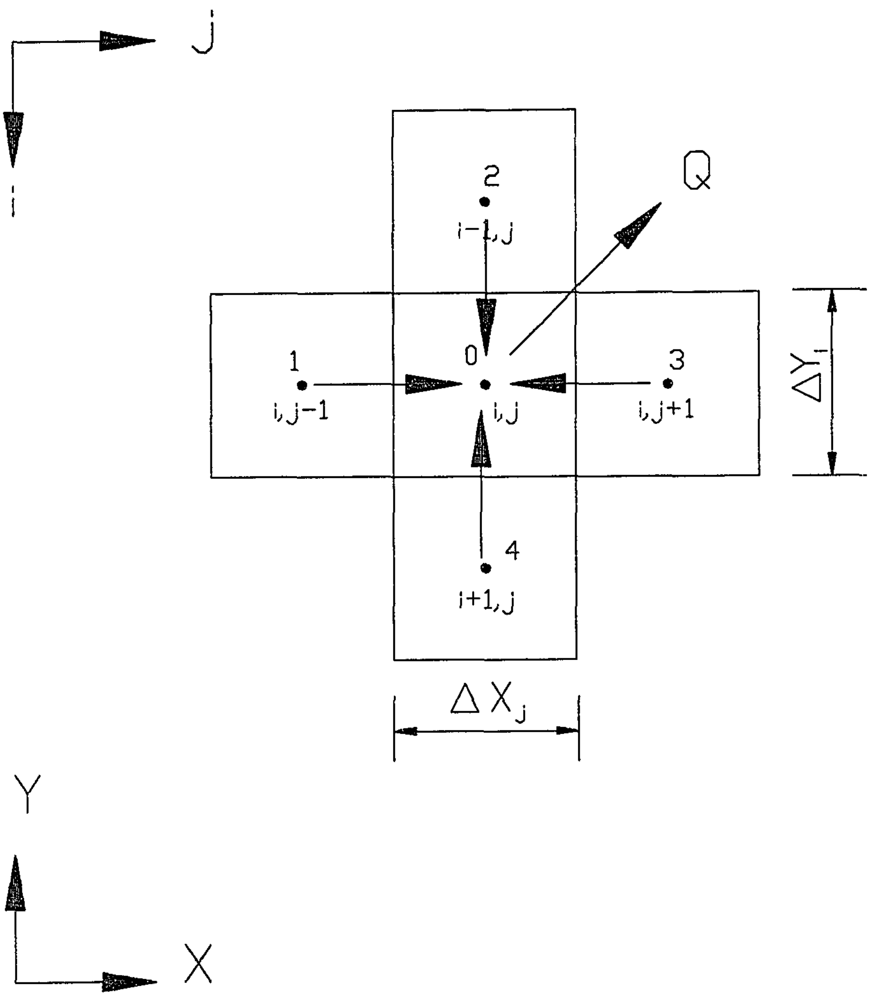


FIG. 3.1: CELL NUMBERING NOTATION IN AQUIFER FLOW USING BLOCK CENTERED FINITE DIFFERENCE GRID

linear equations in tridiagonal form is generated for each individual row of nodes. Row by row, the equations are sequentially generated and solved. This marks the completion of one iterative cycle. This two step process of a iterative cycle is repeated until convergence is achieved.

The convergence criterion defined in the model takes the total system into account by controlling the sum of changes in heads during iterations over the entire model. The sum of changes in heads during iterations should converge to a predefined user specified value. Further to help check the numerical accuracy of the solution obtained mass balance calculations are performed after each time step. The mass balance computed as net inflow (sum of all inflows - sum of all outflows) should equal the change in storage and net recharge from boundaries if any.

The boundary of the aquifer is represented by defining each cell as active (variable head cell), inactive (no flow cell) and constant head or constant flow cell. Leaky conditions, groundwater evapotranspiration, varying areal recharge and induced infiltration from the streams and lakes are taken into account as previously described by Prickett and Lonnquist (1971) and modified where necessary.

3.2.1.1 Unconfined Groundwater Flow Conditions

In unconfined aquifers under non-equilibrium conditions, when subjected to pumping, water is released from storage by the gravity drainage of the interstices resulting in decline of the water table. The unsaturated zone above the water table continues to supply water to the declining water table. Under this condition the coefficient of storage appears to vary and increases at a diminishing rate with the duration of

pumping (Bear, 1972). If pumping continues for sufficiently long time, an asymptotic stage is reached in which a practically constant value of storativity is obtained. Further, if changes in water table elevations or drawdowns are sufficiently small compared with the average depth of flow, Eq. 3.2.1 is applicable to unconfined aquifer flow situations. Thickness of the aquifer, b (in Eq. 3.2.1), is then defined as the average depth of flow, a constant. With these two assumptions linearity of Eq. 3.2.1 is still maintained and the methods discussed under generation of unit-response matrix, and principle of superposition is applicable to unconfined groundwater flow conditions.

3.2.1.2 Leaky Aquifer Conditions

For leaky aquifer conditions, the source term Q_L is evaluated

$$Q_L = \frac{P_{zz_{i,j}} \Delta x_j \Delta y_i}{m_{i,j}} (RH_{i,j} - h_{i,j}^{n+1}) \tag{3.2.3}$$

where, P_{zz} = aquitard permeability, m = aquitard thickness, and RH = source bed or water table elevation, $h_{i,j}$ = piezometric head

3.2.1.3 Groundwater Evapotranspiration

The loss of water due to groundwater evapotranspiration is calculated using

$$Q_{ET} = -ET_{i,j}^{\max} + \frac{ET_{i,j}^{\max}}{(RH'_{i,j} - RD'_{i,j})} (RH'_{i,j} - h_{i,j}^{n+1}) \tag{3.2.4}$$

where, ET^{max} = maximum groundwater evapotranspiration, RH' = ground surface elevation and RD' = the depth below which the evapotranspiration ceases.

3.2.1.4 Areal Recharge

Areal recharge, artificial or natural, is expressed as

$$Q_{AR} = RR_{i,j}\, \Delta x_j\, \Delta y_i \tag{3.2.5}$$

where, RR = areal recharge rate for the cell.

3.2.1.5 Induced Infiltration

The rate of seepage from lakes or streams induced by lowered piezometric surface in the connected aquifer is expressed

$$Q_{INF} = \begin{cases} \dfrac{P'_{zz_{i,j}}\, A_{s_{i,j}}}{m'_{i,j}} \left(hr_{i,j} - h^{n+1}_{i,j}\right), & for\ \ h^{n+1}_{i,j} > hr_b \\[2ex] \dfrac{P'_{zz_{i,j}}\, A_{s_{i,j}}}{m'_{i,j}} \left(hr_{i,j} - hr_{b_{i,j}}\right), & for\ \ h^{n+1}_{i,j} \le hr_b \end{cases} \tag{3.2.6}$$

where, P'_{zz} = stream (lake) bed permeability, m' = bed thickness, A_s = surface area of the stream (lake) in the cell, hr = surface water elevation and hr_b = river bottom elevation. Depending on the surface water elevation and aquifer head h, the induced infiltration Q_{INF} can be either positive or negative, the definitive sketch of Q_{INF} from a stream cell as a function of aquifer piezometric head, h, is shown in Fig. 3.2.

3.3 GENERATION OF SPATIAL RANDOM STOCHASTIC FIELDS

In a heterogeneous and anisotropic medium of the aquifers, the parameters governing the flow process, such as hydraulic conductivity in the X and Y directions, and confined and unconfined storage coefficients are continuously varying in space. Field

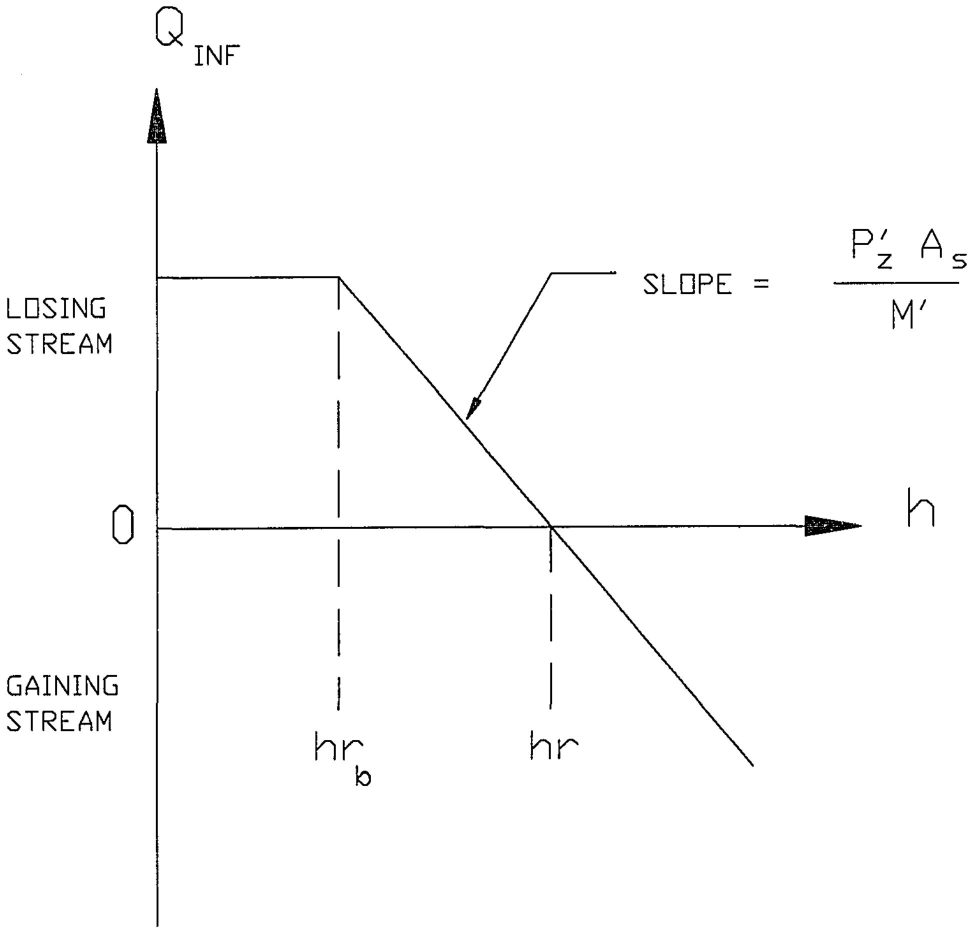


FIG. 3.2: AQUIFER HEAD - INDUCED INFILTRATION RATE CURVE

measurements such as pumping tests are performed to determine the best localized values of these parameters. The values of these different variables at various points are subjected to uncertainty, either because they are generally measured at a limited number of points or because measurements are error prone themselves. Therefore in practice, we typically have sparse data which are inadequate to fully characterize the spatial variability of aquifer parameters. It is in this context, it is recognized that the hydrogeologic parameters be estimated using statistical framework of "theory of estimation".

Although the theory of estimation using statistical methods have long been established, it is only recently that these theories have started penetrating the field of hydrogeology relatively slowly. Further, very little progress is seen in the use of simulation models of stochastic processes for studying the flow and transport process, which ensures a greater degree of reliability while using estimated parameters.

In this work, the following two assumptions are made with respect to hydraulic conductivity in the X and Y directions, and confined and unconfined storage coefficients:

a. The hydrogeologic parameters follow lognormal distribution. The use of logarithms of hydrogeologic parameters as unknown has led to improved parameter estimates due to its following advantages:

    i. It avoids the computation of negative parameter values, and

    ii. It enhances the computational efficiency by improving the rate of convergence.

b. The hydrogeologic parameters are characterized by a stationary exponential covariance function. The hydrogeologic parameters do not have a definite

trend in space. They neither increase nor decrease in any direction systematically. They are unique in space. Hence, the parameters governing the flow and transport processes are defined to be stationary.

These two assumptions are consistent with the findings of Hoeksema and Kitanidis (1985), who analyzed the spatial correlation structure of transmissivity, hydraulic conductivity and storage coefficient using data from 31 aquifers throughout the United States.

Denoting the natural logarithm of a hydrogeologic parameter at any point X_i as Y_i; then under the assumption of stationarity, lognormality and exponential covariance, the mean and covariance for the random log field are:

$$E\,[Y_i] = \mu_Y \tag{3.3.1}$$

$$Q = Cov\ (\xi) = \sigma_Y^2 \exp\left[- \left\{ \left(\frac{\xi_1}{\lambda_1} \right)^2 + \left(\frac{\xi_2}{\lambda_2} \right)^2 \right\}^{\frac{1}{2}} \right] \tag{3.3.2}$$

where, E [ ] denotes expected value, μ_y = mean of the random field, Q = Cov (ξ) = stationary anisotropic exponential covariance for two points separated by vector ξ, σ_Y^2 = variance of the random field, ξ_i = separation along dimensions i (i = 1,2), λ_i = correlation length scale along dimension i. The correlation length is a measure of spatial persistence of zones of similar properties. For example, hydraulic conductivity often is correlated such that values immediately adjacent to one another are similar and those much farther away are dissimilar. This is mainly because of the way in which sediments are deposited.

Based on the measured data, the statistical structural parameters $\mu_y, \sigma_y^2, \lambda_x,$ *and* λ_y are determined using maximum likelihood procedure. The spatial structure of these parameters is the manner in which these variables are correlated and distributed in space.

3.3.1 Maximum Likelihood Estimation (MLE)

Maximum likelihood estimation is widely accepted as one of the most powerful parameter estimation method. In theory and in practice, MLE is primarily applied owing to the following advantages:

a. The method makes use of efficient estimators, and normally distributed (estimators producing minimum variance).

b. The method's estimators are consistent (i.e. with lengths of the samples increasing, the expected values of the parameters estimated from the set of samples converge towards the parameters of the universe).

c. Tests of hypotheses about model structure based upon MLE are optimal for large samples.

d. Distribution of estimation error and test statistics are readily computed.

e. Computation of MLE parameters is a non-linear optimization problem with different methods available to take advantage of sparse matrix structures.

Here, the unknown spatial statistical structural parameters are determined by assuming that the joint probability density function of all measured data is Gaussian. As stated previously, field data suggests this assumption is valid for the logarithm of hydrogeologic parameters.

Under Gaussian assumption, the joint pdf of the measured log parameters is given by:

$$p(Z|\theta) = (2\pi)^{-\frac{N}{2}} |Q|^{-\frac{1}{2}} \exp\{-\frac{1}{2}(Z-\mu)^T Q^{-1} (Z-\mu)\} \tag{3.3.3}$$

where, $p(Z|\theta)$ is called the likelihood function, Z is a vector of measured log parameters, N is the number of measurements; θ is the vector of unknown spatial statistical structural parameters of the log parameter field to be estimated, $|\ |$ denotes determinant, T denotes transpose, μ and Q are the mean and covariance of the measured log parameters given θ. More specifically,

$$\mu = E[Z|\theta] \tag{3.3.4}$$

$$Q = E[(Z-\mu)(Z-\mu)^T|\theta] \tag{3.3.5}$$

The unknown structural parameters are obtained by minimization of the negative log likelihood

$$L(Z|\theta) = -\ln p(Z|\theta) = \frac{N}{2}\ln(2\pi) + \frac{1}{2}\ln|Q| + \frac{1}{2}(Z-\mu)^T Q^{-1}(Z-\mu) \tag{3.3.6}$$

In the above equation, μ and Q are the unknown components, and can be expressed as functions of the unknown structural parameters $\mu_y, \sigma_y^2, \lambda_x,$ *and* λ_y. The optimum value of these unknown structural parameters lie at the extreme of the function, which is obtained by setting the derivative of negative log likelihood function with respect to each of the structural parameters to zero, i.e.,

$$\frac{\partial L}{\partial \mu} = 0; \quad \frac{\partial L}{\partial \sigma^2} = 0; \quad \frac{\partial L}{\partial \lambda_x} = 0; \quad \frac{\partial L}{\partial \lambda_y} = 0 \qquad (3.3.7)$$

Equation 3.3.7 is called the "likelihood equation". $\mu_y, \sigma_y^2, \lambda_x,$ *and* λ_y are obtained by solving the four likelihood equations. A gradient based iterative method called "method of scoring" is employed for minimizing the negative log likelihood function. Details of the computational procedure is given in Appendix A1.

3.3.2 Gaussian Conditional Mean Estimates

In this step, the optimum structural parameters thus obtained is used in estimating the hydrogeologic parameters throughout the aquifer based on the measurement data. Here, the Gaussian conditional mean is used to estimate the average log parameter field, and conditional variance is estimated to quantify the reliability of these estimates.

The Gaussian conditional mean estimate of log parameter at any point i, $\hat{Y}_{GC_i}$, is given by

$$\hat{Y}_{GC_i} = E\,[Y_i|Z] = \mu_Y + Q_{Yiz}\, Q^{-1}\, (Z - \mu) \qquad (3.3.8)$$

where Z = vector of measured log parameters, μ = mean of measured values, Q = covariance of the measured log conductivities and is defined by Eq. 3.3.5, θ = vector of unknown spatial statistical structural parameter of log parameter field to be estimated, and Q_{Yiz} = cross covariance between log parameter at any point i and the measured log parameter.

The conditional variance is estimated to quantify the reliability of these estimates. The conditional variance, $Var[Y_i]$, is given by:

$$Var\ [\hat{Y}_i] = \sigma_Y^2 - Q_{Yiz}\, Q^{-1}\, Q_{Yiz}^T \tag{3.3.9}$$

Once the Gaussian conditional mean estimates, $\hat{Y}_{GC}$, of the log parameters are obtained at all points in the aquifer, conditional simulation is performed to generate multiple realizations of log parameters. The objective of stochastic generation of hydrogeologic parameters is to generate many plausible realizations of these parameters to be used in the simulation-optimization. This will minimize the effects of the uncertainty associated with the governing aquifer flow parameters on model results.

3.3.3 Gaussian Conditional Simulation

Gaussian conditional simulation approach is a classical linear estimation procedure. The advantages are:

a. Conditional simulation is applicable to any type of pdf of the variables of interest.

b. The same concepts as used in Gaussian conditional mean estimates can be applied in conditional simulation and modeling, since we arrive at the entire statistical structure of the variables of interest and not only at the expected value and the covariance.

If Y is the vector of "true" log parameters, then

$$Y = \hat{Y}_{GC} + [Y_u - \hat{Y}_{uGC}] \tag{3.3.10}$$

where, Y_u = vector of unconditional log parameters which has the same statistical properties (i.e. mean and covariance) as Y, $\hat{Y}_{uGC}$ = vector of unconditional log

parameters, based on the same procedure to obtain Gaussian conditional mean estimates, $\hat{Y}_{GC}$. The vector, $\hat{Y}_{uGC}$, is obtained by simply substituting, Z vector of measured log parameters by a vector of unconditional log parameters Y_u (steps involved in obtaining Y_u is discussed below) at the measurement nodes in Eq. 3.3.8.

The steps involved in generating Y_u are

a. Auto-Covariance matrix, $\sum$, is generated using Eq 3.3.2. If there are N cells then the matrix is of order (N x N). This is a positive definite symmetric matrix.

b. Square root of the matrix $\sum$ is obtained such that $\sum^{\frac{1}{2}} \sum^{\frac{1}{2}} = \sum$. This is easily obtained by first determining all the eigen vectors, P, and eigen values, Λ, of the covariance matrix. Then the square root of the covariance matrix is obtained by

$$\sum^{\frac{1}{2}} = P\,\Lambda^{\frac{1}{2}}\,P^{T} \qquad \textbf{(3.3.11)}$$

c. Normal random numbers are generated with mean 0 and variance 1;

$\tilde{U}_i$ = N (0,1)

d. Then Y_u is determined by

$$Y_u = \mu + \sum^{\frac{1}{2}} \tilde{U}_i \qquad \textbf{(3.3.12)}$$

e. Step c is repeated as many times as required to obtain a set of Y_u. For multiple realizations these different sets of Y_u's are used in Eq 3.3.10.

3.3.4 Managing the Size of the Problem

The auto-covariance matrix, $\sum$, is a positive definite symmetric matrix of size (N x N), where N is the number of cells in the aquifer. It was found in the model component developed that the generation of eigen values and eigen vectors of the covariance matrix as the single most process which is computationally intensive and memory intensive. In order to increase the efficiency of the model as applied to, real size problems, an option of dividing the entire domain into regions of smaller autocovariance matrices is developed. When regions are defined, aquifer parameters are generated region by region making use of the measurement nodes in that region and the stochastically generated aquifer parameters assembled in a single vector. One vector for each hydrogeologic parameter for the complete domain for each realization is assembled and stored for further use in flow and transport simulation models.

3.4 UNIT-RESPONSE MATRIX

The two methods which are widely used to accomplish simultaneous management and simulation of groundwater are:

a. Embedding method, and

b. Response matrix method.

Here, the latter method is used, but a brief description of embedding method is also discussed. In general both approaches require that the governing flow equation be discretized using finite differences or finite elements.

In the embedding method the discretized flow equation is "embedded" in the optimization problem along with other constraints that restrict local hydraulic heads,

gradients, and pumping and/or recharge rates. The solution of it results in optimum pumping and injection rates and the response of the entire aquifer in terms of simulated piezometric heads at all the nodes in the system. This approach necessitates that every hydraulic head in the system to be a decision variable in framing the management model. This aspect makes the management model huge, hence in practice this approach is restricted to steady state problems.

In the response matrix approach, the response of the system in terms of change in head at certain key locations (which are of critical interest in managing the system) due to unit excitation at each potential well locations considered separately are recorded as unit-response coefficients. These responses are assembled into a response matrix that is then included in the management model as a set of constraints together with the management and environmental constraints.

3.4.1 Potential Well Locations

In the management of stream-aquifer system for water quantity, it is necessary to identify all the potential well locations. These potential well locations may include all existing well locations together with a set of newly identified well locations. Optimal pumping pattern will then be determined by the management model. By a study of the pumping pattern, one may refine the potential pumping well locations for further study and investigation.

Stream reaches in an aquifer cell is treated in the model as potential well locations. The optimal pumping pattern obtained for stream cells could be either positive

or negative, indicating whether the aquifer is losing water to the stream or gaining water from the stream.

All potential waste disposal injection well sites are treated in the model as potential well locations.

3.4.2 Unit-Response Function, β

In the governing partial differential equation (Eq. 3.2.1), the dependent variable h(x,y,t) does not have any variable coefficients, hence the equation is linear. The advantage of a linear pde is that superposition is allowed.

The change in the aquifer head (drawdowns) over time for a pulse pumping of unit discharge in one time step from each potential well excited separately is recorded as unit-response coefficient, β .

Exact analytical expressions for unit-response function and their proof for a homogeneous, isotropic case is given in Maddock (1972), and separately by Morel-Seytoux (1975). Here, β 's are calculated numerically because no closed form solution exist for their computations. The procedure is as follows:

a. The domain is discretized.

b. To each discrete node, values of hydraulic parameters (conductivity and storativity) are assigned (i.e. taking the values from one realization of aquifer parameters estimated previously or that defined by the user)

c. The initial and boundary conditions are identified and quantified for input into the model.

d. The location of potential wells are designated.

e. Starting from the first well to the last a pumpage of one unit is assigned to that well for the first time step and zero units thereafter.

f. Drawdowns obtained in this manner are the response coefficients - β .

g. For each realization of hydraulic parameters (conductivity and storativity) the above steps are performed and the response coefficients thus obtained are stored separately.

3.4.3 Superposition Using Unit-Response Function

The governing groundwater flow equation (Eq 3.2.1) is linear, the solution, h(x,y,t), can be assembled from the following solution components:

a. Hydraulic heads resulting from initial conditions.

b. Changes in heads due to boundary influences.

c. Changes in heads resulting from the imposed hydraulic stresses, each considered separately.

We can write the above solution components in an equation form as shown below:

Total Head = (Head from Boundary Influences) - (Change in Head Resulting from Initial Conditions) - (Drawdown due to Hydraulic Stresses) (3.4.1)

3.4.3.1 Drawdown due to Hydraulic Stresses

Drawdown due to hydraulic stresses can be computed easily by generating unit-response coefficients as discussed above. In general, drawdown at any point k, within the aquifer for a multiwell system consisting of NW wells and KT time periods for any realization KR is given by

$$s(k,KT) = \sum_{jw=1}^{NW} \sum_{it=1}^{KT} \beta(k,jw,KT-it+1,KR)\ Q_w(jw,it) \qquad (3.4.2)$$

where, s(k,KT) = drawdown at any point k at time step KT, Q_w(jw,it) = pumpage of well jw during period it and β (k,jw,KT-it+1,KR) = system unit response function at point k as a result of unit pumpage at well jw for the $(KT\text{-}it+1)^{th}$ time period, for the realization KR.

It is important to note that this method of stair-stepping the responses due to pumping requires that all pumping periods be of equal length. Since the selection of length of time step is arbitrary, this requirement provides no real drawbacks.

3.4.3.2 Heads due to Boundary Influences

A steady state simulation of the aquifer with no initial conditions and no pumping subjected only to boundary conditions yields heads due to boundary influences.

3.4.3.3 Change in Head Resulting from Initial Conditions

In the generation of unit-response function, it is assumed that the system initially is at rest and the initial piezometric surface is a plane. However, this assumption poses difficulties in dealing with practical problems, where non uniform initial conditions do exist because of prior pumping and/or recharge. Here, in order to overcome this practical difficulty, it is assumed that the system is steady and at rest one time step prior to initial time step. Then stresses which are unknown apriori are applied to the aquifer for one time step that would cause the known initial drawdowns.

The unknown pumping and/or recharge that causes initial drawdowns is computed for each realization by generating unit-response coefficients for one time step.

$$s_{obs}(k) = \sum_{j=1}^{NOBS} s_{\beta}(k,j)\; Q_{init}(j) \tag{3.4.3}$$

where $s_{obs}(k)$ is the known drawdown due to initial conditions at k^{th} observation well, $s_{\beta}(k,j)$ is the unit-response coefficient at the k^{th} observation well due to well pumping at j^{th} observation well, and $Q_{init}(j)$ are the unknown pumping/recharge at the j^{th} pumping well.

The system of equations are solved to obtain the unknown $Q_{init}(j)$, $j = 1,2,...,NOBS$. These are then used in the aquifer simulation in one time step prior to the initial time step either for generating the unit-response coefficient matrix or for just performing simulation.

3.5 SURFACE WATER FLOW COMPONENT

In a connected surface water groundwater system, the analysis of the groundwater flow component described in Section 3.2 is incomplete, if the state variables defining the surface water component namely river stages are not known (ref Eq. 3.2.6). These river stages themselves are an implicit function of the state variables defining the groundwater flow component namely aquifer heads. In the simulation-optimization procedure developed here for the conjunctive-use management of connected surface water groundwater systems, the analysis and management of surface water flow component are embedded in the management model together with the unit-response function obtained for groundwater flow component.

Here the hydraulic and hydrologic equations used in the analysis of the surface water flow component are discussed.

3.5.1 Hydraulic Equations

The discharge-area relationship for streams is often expressed by

$$Q = \alpha_1 A^{\beta_1} \tag{3.5.1}$$

where, Q = discharge, A = cross-sectional flow area, α_1 and β_1 are constant parameters.

The depth-area relationship for the cross-section of a stream reach can be expressed in a similar form to Eq. 3.5.1 and is given by

$$A = \alpha_2 y^{\beta_2} \tag{3.5.2}$$

where, y is the stream depth in the reach, α_2 and β_2 are constant parameters.

Combining Eq. 3.5.1 and Eq. 3.5.2, the stage-discharge relationship can be expressed in the form as

$$Q = \alpha_1 (\alpha_2)^{\beta_1} y^{\beta_1 \beta_2} \tag{3.5.3}$$

These relationships can be obtained from the rating curve of a channel. If these relationships are not available readily and only discharge-area and area-depth measurements are made available, then the model computes the constant parameters α_1, β_1, α_2 , and β_2 using least square analysis, and expressed as

$$\alpha_1 = 10^{\frac{\sum \log Q - \beta_1 \sum \log A}{N}} \tag{3.5.4}$$

$$\beta_1 = \frac{\left[\sum (\log Q)\ (\log A)\right] - \left(\frac{\sum \log Q \sum \log A}{N}\right)}{\sum (\log A)^2 - \frac{\left(\sum \log A\right)^2}{N}} \tag{3.5.5}$$

where, N is the number of measurements of Q and A. On similar lines constant parameters of Eq. 3.5.2 is determined, if measurements are made available.

If the rating curve or the actual measurements are unavailable, assumption of wide rectangular channel is made. The constant parameters are then obtained by using the Manning formula as

$$\alpha_1 = \frac{86400\ S_o^{\frac{1}{2}}}{n\ T_w^{0.667}} \tag{3.5.6}$$

$$\beta_1 = 1.67 \tag{3.5.7}$$

$$\alpha_2 = T_w \tag{3.5.8}$$

$$\beta_2 = 1.0 \tag{3.5.9}$$

where, S_o is the bed slope (an approximation for the unknown friction slope, S_f), n is the roughness coefficient, T_w is the top width of the reach. When constant parameters or measurement values are input to the model, top width T_w is calculated by

$$T_w = \frac{\partial A}{\partial y} = \alpha_2 \, \beta_2 \, y^{\beta_2 - 1} \tag{3.5.10}$$

3.5.2 Hydrologic Storage Equation

The hydrologic storage equation for a stream/channel reach is given by

$$\frac{dS}{dt} = Q_{u/s} - Q_{d/s} - Q_{SWD} \pm Q_{INF} + Q_{WD} \tag{3.5.11}$$

where, S = volume of water in storage in the channel reach, $Q_{u/s}$ = upstream inflow rate, $Q_{d/s}$ = downstream outflow rate, Q_{SWD} = surface water diversion from the reach, Q_{INF} = gain or loss into the stream reach due to induced infiltration, t = time, Q_{WD} is the waste disposal rate into the stream reach.

3.5.3 Finite Difference Equation

Fig 3.3 shows the cell numbering notation used in the block centered finite difference grid of the one-dimensional stream flow. For any time increment, Δt , the finite difference form of the Eq 3.5.11 is expressed as

$$\begin{aligned} \frac{S_i^{n+1} - S_i^n}{\Delta t} &= \frac{Q_{i-\frac{1}{2}}^n + Q_{i-\frac{1}{2}}^{n+1}}{2} - \frac{Q_{i+\frac{1}{2}}^n + Q_{i+\frac{1}{2}}^{n+1}}{2} \\ &- \frac{Q_{SWD_i}^n + Q_{SWD_i}^{n+1}}{2} \pm \frac{Q_{INF_i}^n + Q_{INF_i}^{n+1}}{2} + \frac{Q_{WD_i}^n + Q_{WD_i}^{n+1}}{2} \end{aligned} \tag{3.5.12}$$

Expressing storage S of a reach in terms of y, yields

$$S_i = L_i \, A_i = L_i \left(\alpha_2 \, y_i^{\beta_2} \right) \tag{3.5.13}$$

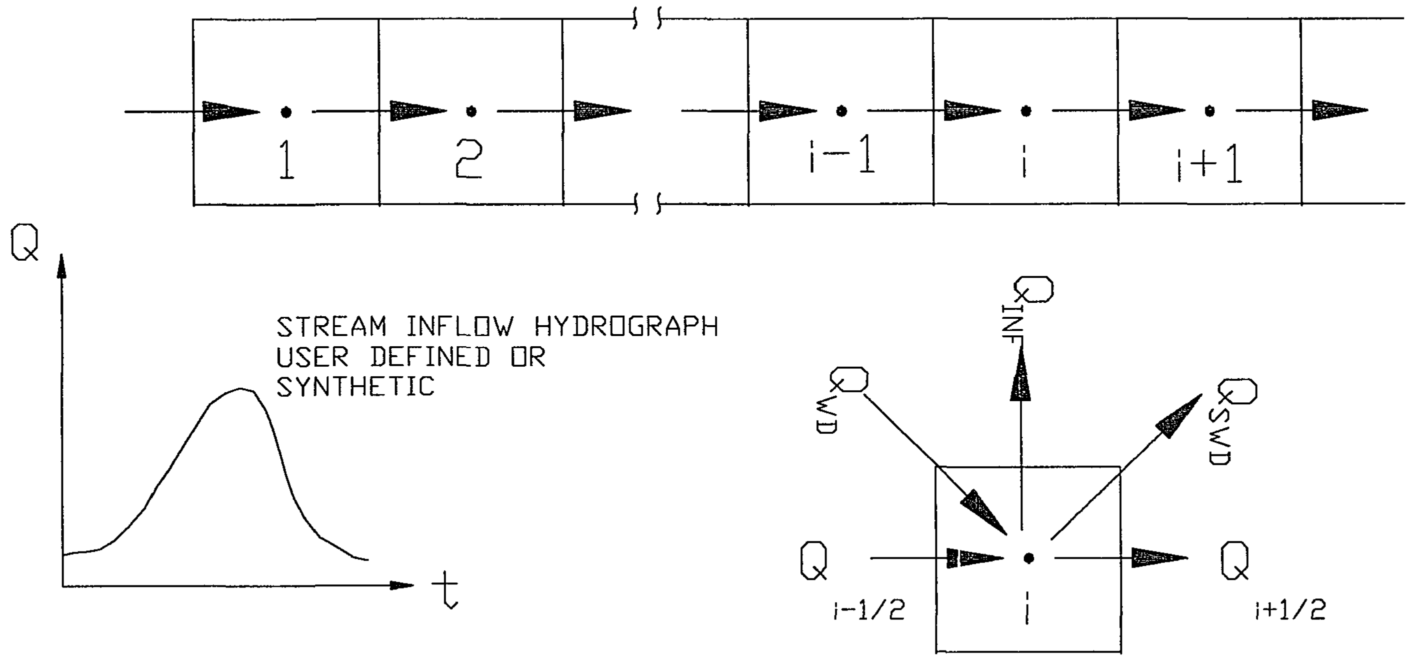


FIG. 3.3: CELL NUMBERING NOTATION FOR
ONE-DIMENSIONAL STREAM FLOW

Using Eq 3.5.3, upstream inflow ($Q_{i-1/2}$) and downstream outflow ($Q_{i+1/2}$) of a reach is expressed in terms of flow depth, y as

$$Q_{i-\frac{1}{2}} = \alpha_1 \, (\alpha_2)^{\beta_1} \, y_{i-1}^{\beta_1\beta_2} \tag{3.5.14}$$

$$Q_{i+\frac{1}{2}} = \alpha_1 \, (\alpha_2)^{\beta_1} \, y_{i}^{\beta_1\beta_2} \tag{3.5.15}$$

For the first reach the upstream inflow rate can be either a user specified hydrograph or a synthetic hydrograph generated (discussed in Section 3.5.4).

The induced infiltration, Q_{INF}, is an implicit function of river head, hr, and aquifer head in the river cell. The implicit expression used is

$$Q_{INF}^{n} = \frac{P'}{m} As_i \left(hr_i^{n} - ha_i^{n}\right) \tag{3.5.16}$$

where, river head $hr = y + hr_b$, hr_b is the river bed elevation in the reach, y is the stream flow depth, n is the time step, and the aquifer head in the river reach i, ha, for the realization KR is given by

$$\begin{aligned} ha^{n} = h_o &- \left[\sum_{it=1}^{n} \sum_{jw=1}^{NW} \beta(i,jw,n-it+1,KR)\; Q_w(jw,it)\right] \\ &+ \left[\sum_{it=1}^{n} \sum_{ir=1}^{NR} \beta(i,ir,n-it+1,KR)\, Q_{INF}(ir,it)\right] \end{aligned} \tag{3.5.17}$$

Substituting Eq 3.5.17 in Eq 3.5.16 gives the implicit equation in Q_{INF}. The solution is obtained in the management model by setting the implicit equation as a strict equality constraint as discussed in Section 3.10. Further, Eq. 3.5.13 through Eq. 3.5.16 are substituted in the finite difference equation Eq. 3.5.12, yielding only stream depth, y,

surface water diversion, Q_{SWD}, aquifer head, h, as unknown. Eq. 3.5.12 is a strict non-linear equation. In the management model (to be discussed later) this Eq 3.5.12 is set as a non-linear equality constraint.

3.5.4 Stochastic Streamflows

In the surface water flow component the upstream inflow of the stream could be either a user specified hydrograph or a synthetic hydrograph. Synthetic streamflows help evaluate the sensitivity of the proposed conjunctive-use management designs of a regional system more thoroughly and in a statistically sophisticated manner. If the historical streamflow record is available, the model developed can generate a synthetic hydrograph.

3.5.4.1 Statistics of Observed Flows

The historical streamflow record provides some valuable insight to the future behavior of that stream. To generate a sequence of values of synthetic flows for a given stream, flows are considered to be the results of a random process. The generated sequence, however, must possess the same characteristics of mean, variance, skewness, and serial correlation as the observed flows.

If N is the size of the sample of the historical record, then the mean, $\bar{Q}$, is computed as

$$\bar{Q} = \frac{1}{N}\sum_{i=1}^{N} Q_i \tag{3.5.18}$$

The spread of the historical record as measured by its variance and is computed as

$$\sigma^2 = \frac{1}{N-1}\left(\sum_{i=1}^{N} Q_i^2\right) - \frac{N}{N-1}\bar{Q}^2 \tag{3.5.19}$$

The dimensionless coefficient of skewness measures the degree of symmetry (or really the lack of it) of the distribution about its mean. The coefficient of skewness for a symmetric distribution is, $\gamma = 0$. Here in this research work, a normal or log-normal type of distribution is used for generation of synthetic streamflows. Coefficient of skewness (is calculated for both types of distribution) is used as a decisive factor in selecting the type of distribution. The coefficient of skewness is computed as

$$\gamma = \frac{\sum_{i=1}^{N} Q_i^3 - 3\bar{Q}\sum_{i=1}^{N} Q_i^2 + 2N\bar{Q}^3}{N\left(\frac{1}{N}\sum_{i=1}^{N} Q_i^2 - \bar{Q}^2\right)^{\frac{3}{2}}} \tag{3.5.20}$$

In general it is found from analysis of historical flow records that the observed streamflows have a high degree of persistence (Fiering and Jackson, 1971). That is, typically a low flow is more likely to be followed by another low flow rather than a high flow. Similarly a high flow is more likely to be followed by another high flow.

In order to incorporate this flow persistence in the stochasitically generated streamflows it is found sufficient to expect flow in one time step to be dependent on the flow in the previous time step. However, if the length of the sample (observed flows) is large enough one may consider the flows to lag differently. For this the lag-k serial correlation coefficient is computed as

$$r_k = \frac{\sum_{i=1}^{N-k} Q_i \, Q_{i+k} - \frac{1}{N-k}\left(\sum_{i=1}^{N-k} Q_i\right)\left(\sum_{i=k+1}^{N} Q_i\right)}{\left[\sum_{i=1}^{N-k} Q_i^2 - \frac{1}{N-k}\left(\sum_{i=1}^{N-k} Q_i\right)^2\right]^{\frac{1}{2}} \left[\sum_{i=k+1}^{N} Q_i^2 - \frac{1}{N-k}\left(\sum_{i=k+1}^{N} Q_i\right)^2\right]^{\frac{1}{2}}} \qquad (3.5.21)$$

where, Q_i = vector of historical streamflows, $\bar{Q}$ = mean or average of the vector Q_i, N = size of the sample, σ^2 = variance, k = lag, r_k = lag k serial correlation coefficient.

3.5.4.2 Generation of Synthetic Streamflows

The selection of the type of distribution, whether normal or log-normal, facilitates the synthetic generation of streamflows by a Markov model. The generating equation is

$$Q_i' = \bar{Q} + r_1 \left(Q_{i-1}' - \bar{Q}\right) + t_i \, \sigma \sqrt{1-r_1^2} \qquad (3.5.22)$$

where, Q_i' = synthetic streamflows, σ = standard deviation (= $\sqrt{\sigma^2}$), t_i = independent normal sampling deviates with mean 0 and variance 1, and r_1 is the lag-one serial correlation coefficient.

The above equations (Eq 3.5.18 through Eq 3.5.21) are applicable to flows that are normally distributed, and Eq 3.5.22 generates synthetic flows that are normally distributed. Likewise, for log-normal distribution, logarithms of observed flows are used in Eq 3.5.18 through Eq 3.5.21 and Eq 3.5.22 generates a sequence of logarithms of flows that are log-normally distributed.

3.6 GROUNDWATER SOLUTE TRANSPORT COMPONENT

So far, only the development of groundwater and surface water flow component are discussed. The main thrust of this research lies in the overall development and management of a water resources system, including that of water quality.

From the perspective of groundwater pollution, the most important characteristic is the concentration of the solute. The dissolved concentration is defined as mass of solute (or pollutant) that will dissolve in unit volume of water. In the solute transport model developed here, only a single chemical component is considered. Further, the model is limited to transport of solute only in the saturated zone. The reason for this limitation is that the transport of pollutants in unsaturated zone is essentially limited to vertical transport between ground level and top of saturated zone. Also, the long range spreading of pollutants is only possible in the saturated zone, where the dissolved pollutants are carried by the prevailing flow mainly in the horizontal direction.

In this section, the methodology used in modeling the transport process is discussed. The groundwater solute transport component is based on the advection-dispersion equation describing movement of pollutants in a porous medium.

3.6.1 Transport Equation

The main mechanisms affecting the transport of a solute in a porous medium are: advection, mechanical dispersion, molecular diffusion, solid-solute interaction, and various chemical reactions, and decay phenomena together with external sources and/or sinks. Here, all the mechanisms except for solid-solute interaction and

complex chemical reactions are considered. Further, it is assumed that the constituent dissolves fully in water but the flow of groundwater is not affected by density changes.

The unsteady, two-dimensional, advection-dispersion equation describing the transport of solutes in aquifers with first-order decay and external sources and/or sinks is given by:

$$\frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right) - \frac{\partial}{\partial x}\left(K_x \frac{\partial h}{\partial x} C\right) - \frac{\partial}{\partial y}\left(K_y \frac{\partial h}{\partial y} C\right) \pm C_w' W - d_k C = \phi \frac{\partial C}{\partial t} \tag{3.6.1}$$

where, K_x and K_y = hydraulic conductivities, D_x and D_y = dispersion coefficients in the X and Y directions, respectively, C and C_w' = concentration in the aquifer and that of solute in the source or sink fluid respectively, h = piezometric head obtained from the flow equation, W = volumetric flux per unit volume, d_k = reaction coefficient, ϕ = porosity, and t = time.

In order to solve Eq. 3.6.1 appropriate initial and boundary conditions in the X and Y directions are needed to obtain a unique set of solution. The initial distribution of concentration within the porous medium constitutes the initial condition. The boundary conditions are usually specified in terms of prescribed concentration (Dirichlet type) or prescribed boundary flux (Neumann type).

In all the literature reviewed so far, researchers in their work have considered the above pde linear as their velocity distribution is a constant. Strictly speaking the above pde is non-linear. The non-linearity arises form the fact that the velocity distribution throughout the aquifer is a function of space and time. However, the

above pde can be considered linear within each time step individually provided the piezometric head distribution is known throughout the aquifer. In order to provide a known piezometric head distribution for each time step, at first the flow processes described under groundwater flow component and surface water flow component are integrated, and a management problem is formulated and solved to maximize system output. The actual piezometric head distributions are computed for each time step throughout the aquifer by executing the simulation program with known optimal well pumpages from optimal well locations, and optimal surface water diversions. The details of the optimization procedure are described later.

The first two terms on the left hand side of the equation describes the dispersive component of solute transport. Dispersion is the result of two processes, molecular diffusion and mechanical mixing. Diffusion is the process whereby molecular constituents move under the influence of their kinetic activity in the direction of their concentration gradients. While, the mechanical mixing component of the dispersion process is the result of velocity variations within the porous medium. Mechanical mixing and molecular diffusion are referred to collectively as hydrodynamic dispersion or just dispersion. The dispersion serves to spread the contaminant plume over a greater area (both parallel and orthogonal to the hydraulic gradient) than would be occupied if only advection was occurring. In heterogeneous aquifers the irregularities of the flow paths increases, thereby a subsequent increase in spread of the contaminant. It is this heterogenous nature of the aquifer that makes the dispersion process as important as advection in the transport mechanism. The dispersion as described above is a complex process by itself, but yields to better modeling procedures without complications.

The next two terms on the left hand side of the equation describes the advective component of solute transport process. Advection describes mass transport due simply to the flow of water in which the mass is dissolved. The direction and rate of transport coincides with that of groundwater flow. Advective component in general is a more important transport process and is better understood but poses difficulty in accurate modeling.

The methodology developed here in the numerical simulation of transport, for clarity, is discussed separately for the two basic mechanisms - dispersion and advection governing the solute transport in aquifers.

3.6.2 Dispersion Component

Dispersive fluxes entering a finite difference cell from all the four sides is considered in writing expression for mass conserving over the element (ref Fig 3.4). Defining

$$Dxx1 = Dxx_{i,j-1}\ \Delta y_i \left(\frac{b_{i,j}+b_{i,j-1}}{\Delta x_{j-1}+\Delta x_j} \right) \tag{3.6.2}$$

$$Dxx3 = Dxx_{i,j+1}\ \Delta y_i \left(\frac{b_{i,j}+b_{i,j+1}}{\Delta x_{j+1}+\Delta x_j} \right) \tag{3.6.3}$$

$$Dyy2 = Dyy_{i-1,j}\ \Delta x_j \left(\frac{b_{i,j}+b_{i-1,j}}{\Delta y_{i-1}+\Delta y_i} \right) \tag{3.6.4}$$

$$Dyy4 = Dyy_{i+1,j}\ \Delta x_j \left(\frac{b_{i,j}+b_{i+1,j}}{\Delta y_{i+1}+\Delta y_i} \right) \tag{3.6.5}$$

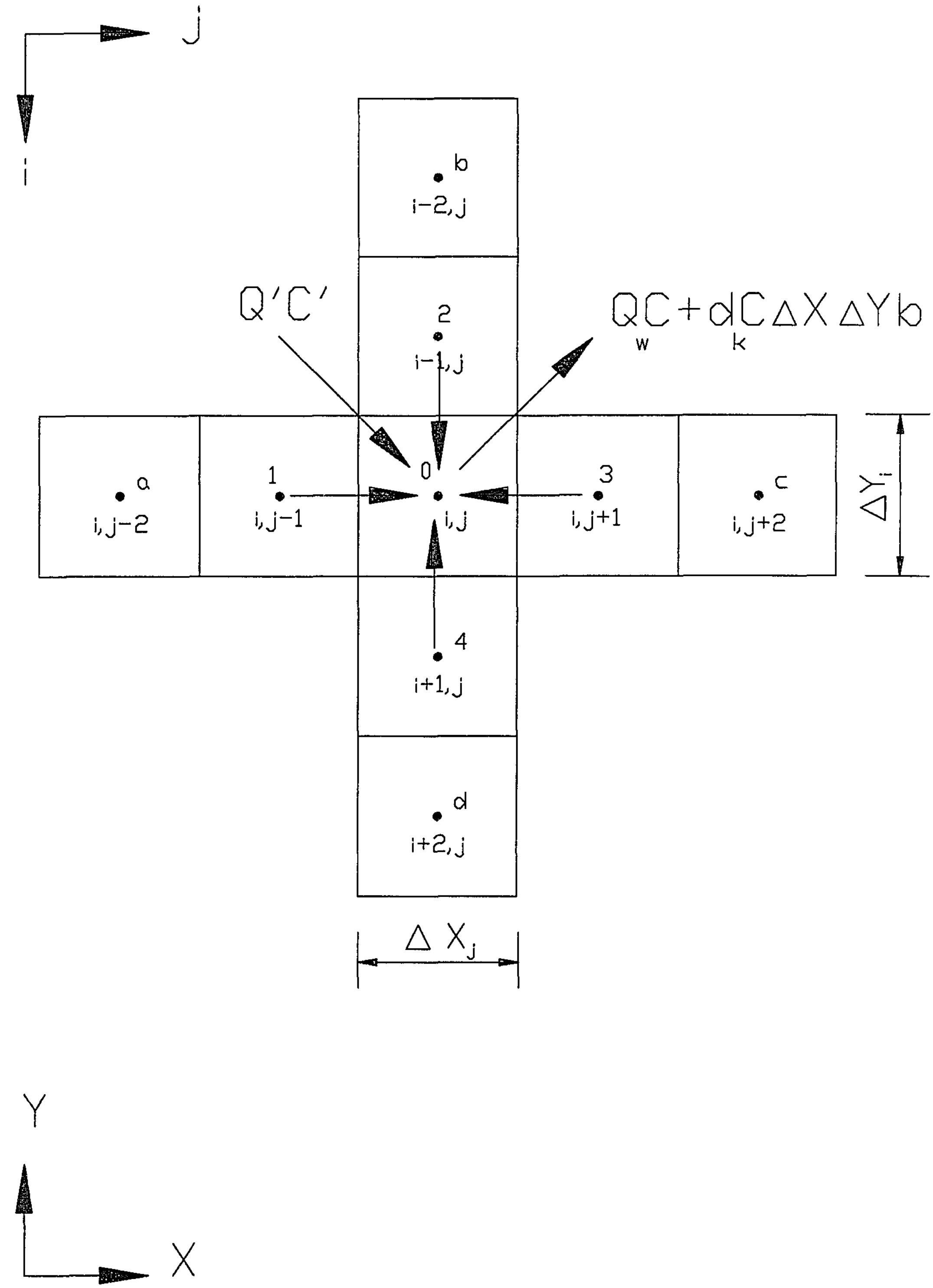


FIG. 3.4: CELL NUMBERING NOTATION USED FOR SOLUTE TRANSPORT IN GROUNDWATER

Dispersive input in X direction entering the Cell (i,j) from left face

$$= Dxx1\ (C_{i,j-1} - C_{i,j}) \tag{3.6.6}$$

Dispersive input in X direction entering the Cell (i,j) from right face

$$= Dxx3\ (C_{i,j+1} - C_{i,j}) \tag{3.6.7}$$

Dispersive input in Y direction entering the Cell (i,j) from top face

$$= Dyy2\ (C_{i-1,j} - C_{i,j}) \tag{3.6.8}$$

Dispersive input in Y direction entering the Cell (i,j) from bottom face

$$= Dyy4\ (C_{i+1,j} - C_{i,j}) \tag{3.6.9}$$

In the computation of groundwater solute transport component, the piezometric heads obtained from the flow simulation is used to define velocities $Uxx_{i,j}$ and $Uyy_{i,j}$ throughout the grid for each time step (ref Fig. 3.5). In the figure Uxx is the groundwater velocity in the X direction calculated between nodes (i,j) and (i,j+1). Similarly, Uyy is the groundwater velocity in the Y direction calculated between nodes (i,j) and (i-1,j). The velocities $Uxx_{i,j}$ and $Uyy_{i,j}$ are defined at the right face and top face of each finite difference cell, and expressed by:

$$Uxx_{i,j} = \left(\frac{Kx_{i,j} + Kx_{i,j+1}}{2}\right) \frac{h_{i,j} - h_{i,j+1}}{\left(\frac{\Delta x_j + \Delta x_{j+1}}{2}\right)} \tag{3.6.10}$$

Similarly,

$$Uyy_{i,j} = \left(\frac{Ky_{i,j} + Ky_{i-1,j}}{2}\right) \frac{h_{i,j} - h_{i-1,j}}{\left(\frac{\Delta y_i + \Delta y_{i-1}}{2}\right)} \tag{3.6.11}$$

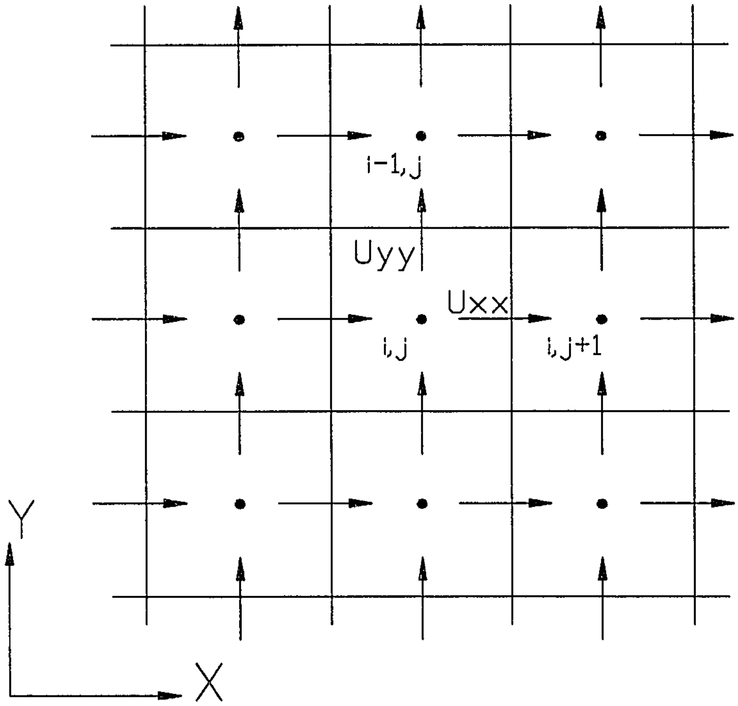


FIG. 3.5: DEFINITION SKETCH OF INTERNODAL VELOCITIES

In the case of uniform flow field a well established linear relationship exists between coefficient of hydrodynamic dispersion and linear groundwater velocity. For the non-uniform flow field considered here, the linear relationship is extended to account for velocity components in the X and Y directions. In the calculations of dispersion coefficient on the grid, velocities between nodes or averages thereof are used. Interpolation of velocities used in the calculation of dispersion coefficient is shown in the Fig. 3.6. In the figure Uxy is the interpolated velocity in the Y direction on the right face of the cell, and Uyx is the intepolated velocity in the X direction on the top face of the cell.

Dispersion coefficient in x direction is defined as

$$Dxx_{i,j} = \frac{\alpha_L\, Uxx^2 + \alpha_T\, Uxy^2}{U} \tag{3.6.12}$$

With Uxx = $Uxx_{i,j}$, and

$$Uxy = \frac{Uyy_{i+1,j} + Uyy_{i,j} + Uyy_{i,j+1} + Uyy_{i+1,j+1}}{4} \tag{3.6.13}$$

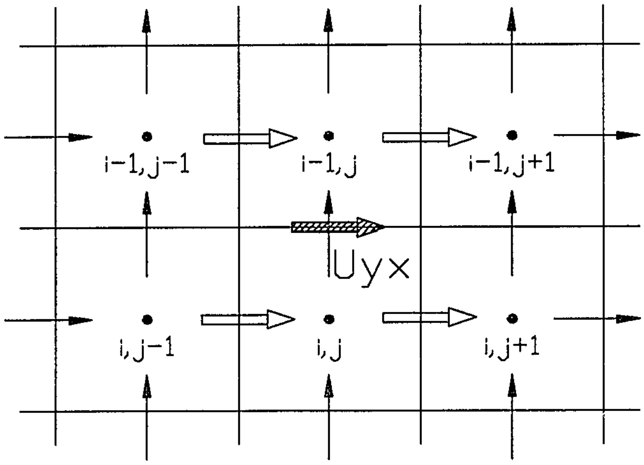
$$U = \sqrt{Uxx^2 + Uxy^2} \tag{3.6.14}$$

Dispersion coefficient in y direction is defined analogously as

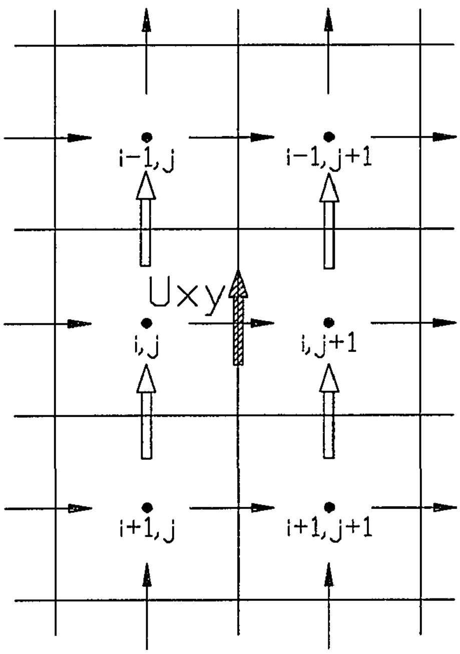
$$Dyy_{i,j} = \frac{\alpha_T\, Uyx^2 + \alpha_L\, Uyy^2}{U} \tag{3.6.15}$$

With Uyy = $Uyy_{i,j}$, and

$$Uyx = \frac{Uxx_{i-1,j-1} + Uxx_{i-1,j} + Uxx_{i+1,j-1} + Uxx_{i,j}}{4} \tag{3.6.16}$$



(a) Internodal velocities used in interpolation of Uyx



(b) Internodal velocities used in interpolation of Uxy

FIG. 3.6: INTERPOLATION OF VELOCITIES USED IN CALCULATION OF DISPERSION COEFFICIENTS

$$U = \sqrt{Uyx^2 + Uyy^2} \qquad (3.6.17)$$

In general it is found where advection dominates dispersion the concentrations in four direct neighbors are sufficient to calculate dispersive fluxes into cell (i,j). There is no need to compute off diagonal elements of the dispersion tensor namely dispersive input in the X direction due to concentration gradient in the Y direction and dispersive input in the Y direction due to concentration gradient in the X direction, as they are insignificant in a advective dominated flow process.

3.6.3 Advective Component

There are numerous schemes available to model advective transport. Several schemes were investigated for use in this research work. In the computation of mass balance of advective fluxes into and out of a cell (i,j) on all four sides of a finite difference cell, the concentration is combined with velocity. The difficulty arises in accurately representing the cell wall concentrations. To this effect four different schemes are included here, and the user has the option of selecting any one of the four schemes.

a. Central Difference Scheme.

b. Upwind Difference Scheme.

c. Weighted Upwind Difference Scheme.

d. Quadratic Upstream Interpolation Scheme.

Each of these schemes has its merits and drawbacks as will be discussed later.

3.6.3.1 Weighted Upwind Difference Schemes

Here the first three schemes are integrated to act as one weighted upwind difference scheme, as upwind difference (with upstream weight of 1.0) and central difference (with upstream weight of 0.5) are special cases of weighted upwind difference scheme. The general expression for determining the cell wall concentration has the form

$$C_{i,j+\frac{1}{2}} = W\, C_{i,j+1} + (1-W)\; C_{i,j} \qquad (3.6.18)$$

with weight W being $0.5 \leq W \leq 1.0$, if the fluid flows from node (i,j+1) to node (i,j). Where $C_{i,j+1/2}$ = cell wall concentration, $C_{i,j+1}$= concentration at node (i,j+1), and $C_{i,j}$ = concentration at the node (i,j).

In the central difference scheme weight W = 0.5. Therefore, the interface concentration is set equal to average of the concentration of the two adjacent nodes to the cell wall: that is $C_{i,j\pm\frac{1}{2}} = 0.5\ (C_{i,j\pm 1} + C_{i,j})$. The space truncation approximation of this advective term by the central differencing scheme is correct to second-order. It is observed, that central differencing leads to unphysical oscillations in an implicit solution scheme where advection dominates dispersion. Physically speaking, the advective flux carries solute downstream aided by the flow velocity. Because of this nature, the cell wall concentration will have a concentration closer to upstream value, this effect is not reflected when using central difference scheme.

In the upwind difference scheme weight W = 1.0. Therefore the interface concentration is set equal to the upstream value: that is $C_{i,j+1/2} = C_{i,j+1}$ if the fluid flows from node (i,j+1) to node (i,j). In other words, a backward difference, $C_{i,j+1}$ - $C_{i,j}$, is used for the advective term at node (i,j). The upwind difference eliminates the oscillations

present in the central difference scheme. They introduce, in turn, a space discretization error, called artificial or numerical dispersion, which produces the same effect as physical dispersion. The magnitude of this numerical dispersion is graphically shown in Section 4.4 under model verification.

Although, in principle, grid refinement can alleviate all these problems (error of numerical dispersion in upwind difference scheme and the error of numerical oscillations in central difference scheme), the necessary degree of refinement is often totally impracticable for engineering purposes, especially if one is attempting to model a regional aquifer which extends to several ten's of kilometers. The general upstream weighted difference method included here, minimizes these problems without going into a costly, impracticable grid refinement.

The mass of solute transported by way of advection is a product of flow and concentration entering the Cell (i,j) through each of the four faces (ref Fig 3.4). The flow term in the advective component can be written as follows

Flow entering the aquifer from the left face

$$T1 = + Uxx_{i,j-1} \, \Delta y_i \left(\frac{b_{i,j} + b_{i,j-1}}{2} \right) \tag{3.6.19}$$

Flow entering the aquifer from the right face

$$T3 = - Uxx_{i,j} \, \Delta y_i \left(\frac{b_{i,j} + b_{i,j+1}}{2} \right) \tag{3.6.20}$$

Flow entering the aquifer from the top face

$$T2 = - Uyy_{i,j} \, \Delta x_j \left(\frac{b_{i,j} + b_{i-1,j}}{2} \right) \tag{3.6.21}$$

Flow entering the aquifer from the bottom face

$$T4 = + Uyy_{i+1,j}\ \Delta x_j \left(\frac{b_{i,j} + b_{i+1,j}}{2} \right) \tag{3.6.22}$$

Advective component in X direction, for mass entering the Cell (i,j) from left face $= T1\ (\ W_a\ C_{i,j-1} + (1 - W_a)\ C_{i,j}\ )$ (3.6.23)

Advective component in X direction, for mass entering the Cell (i,j) from right face $= T3\ (\ W_c\ C_{i,j+1} + (1 - W_c)\ C_{i,j}\ )$ (3.6.24)

Advective component in Y direction, for mass entering the Cell (i,j) from top face $= T2\ (\ W_b\ C_{i-1,j} + (1 - W_b)\ C_{i,j}\ )$ (3.6.25)

Advective component in Y direction, for mass entering the Cell (i,j) from bottom face $= T4\ (\ W_d\ C_{i+1,j} + (1 - W_d)\ C_{i,j}\ )$ (3.6.26)

where W_a, W_b, W_c, and W_d are the weights associated on the left, top, right, and bottom faces, respectively.

As in the case of groundwater flow component, the block centered finite difference formulation for dispersive component and weighted upwind difference formulation for advective component for the governing advection-dispersion equation given in Eq. 3.6.1, follows from the application of continuity of mass: sum of all mass flow rates into and out of a Cell (i,j) that has sides Δx_j and Δy_i must equal rate of change of mass in the aquifer element (ref Fig 3.4).

$$
\begin{aligned}
& Dxx1\,(C^{n+1}_{i,j-1} - C^{n+1}_{i,j}) + Dxx3\,(C^{n+1}_{i,j+1} - C^{n+1}_{i,j}) + \\
& Dyy2\,(C^{n+1}_{i-1,j} - C^{n+1}_{i,j}) + Dyy4\,(C^{n+1}_{i+1,j} - C^{n+1}_{i,j}) + \\
& T1\,(W_a C^{n+1}_{i,j-1} + (1-W_a)\,C^{n+1}_{i,j}) + T3\,(W_c C^{n+1}_{i,j+1} + (1-W_c)\,C^{n+1}_{i,j}) + \\
& T2\,(W_b C^{n+1}_{i-1,j} + (1-W_b)\,C^{n+1}_{i,j}) + T4\,(W_d C^{n+1}_{i+1,j} + (1-W_d)\,C^{n+1}_{i,j} - \\
& d_k(\phi\, b_{i,j}\Delta x_j\ \Delta y_i)\,C^{n+1}_{i,j} + C'_{i,j}Q'_{i,j} - Qw_{i,j}C^{n+1}_{i,j} \\
& \qquad = (\phi\, b_{i,j}\Delta x_j\ \Delta y_i)\left(\frac{C^{n+1}_{i,j} - C^{n}_{i,j}}{\Delta t}\right)
\end{aligned}
\tag{3.6.27}
$$

where ϕ is the aquifer porosity, d_k is the decay rate [1/T], Q_w is the groundwater pumping associated with the node (i,j), C' and Q' are the concentration and waste discharge rate of the external sources, n is the time step, and Δt = length of the time step.

As can be seen from the above equation, the transport model has two state variables: the hydraulic head, h(x,y,t), and the solute concentration, C(x,y,t). In all the literature reviewed so far for management of water quality, the flow model is restricted to steady-state flow so that h is a function only of space, enabling them to treat the transport equation as a linear pde. In the model developed here, the flow model is not restricted to steady-state flow, and the practical approach for treating the transport equation as a linear pde is discussed later in this report.

The solution of the advection-dispersion finite difference equation is obtained by IADI method.

3.6.3.2 Quadratic Upstream Interpolation Scheme

The methods described above to model the advective component usually results in qualitatively acceptable solutions. As discussed later in this report under Model

Verification, these methods have produced global correspondence with measured results. It can be said, for a preliminary engineering analysis these methods are useful. However, in the situations where groundwater pumping creates high gradients, the advective transport is often the most critical process. Under these circumstances, it would be disconcerting to let numerical inaccuracies to dominate the transport process.

The only problem seen in accurate modeling of advective component of the transport process is the method of estimating the interface values of the concentration in the control-volume approach used here. In order to avoid numerical oscillations of central differencing and still remaining free of numerical dispersion associated with upwind differencing, here a stable and accurate method is developed based on quadratic upstream interpolation. In this method, the interface concentration is written in terms of quadratic interpolation using the concentration values of two adjacent nodes to the interface together with the value at the next upstream node. For one-dimensional, steady and unsteady situations Leonard (1979) gives a full description of quadratic upstream interpolation method and demonstrates its numerical stability. Abbott and Basco (1990) gives a brief description of the quadratic upstream interpolation method used by Leonard.

The development of quadratic upstream interpolation scheme for a non-uniform two-dimensional grid and the general computational procedure involved are given in Appendix A2. The comprehensive computer programming flow chart developed for aquifer flow and transport simulation is given in Appendix A3. Here, only a brief description of modeling the advective component using quadratic upstream interpolation scheme and the finite difference formulation for the advection-dispersion equation are given.

With reference to Fig. 3.7, $C_{f\,u/s}$, $C_{u/s}$, and $C_{d/s}$ stand for concentration at far upstream node, upstream node, and downstream node, respectively. For breivity hereafter they are referred to as C_f, C_u, and C_d, respectively. Also, Δ_f is the distance between the far upstream node and upstream node, and Δ_u is the distance between the upstream node and downstream node. Further, Z can either take X dimension or Y dimension.

The most general quadratic interpolation function with two adjacent nodal concentration to the cell wall under consideration together with one upstream node concentration is given by

$$f = W_{d/s}\, C_d + W_{u/s}\, C_u + W_{f\,u/s}\, C_f \tag{3.6.28}$$

where f is the quadratic interpolation function, and the weights associated to the downstream, $W_{d/s}$, upstream, $W_{u/s}$, and far upstream, $W_{f\,u/s}$, nodes are expressed by

$$W_{d/s} = \frac{\Delta_f\, Z^2 - \Delta_f^2\, Z}{\Delta_f\, (\Delta_u^2 + \Delta_f \Delta_u)} \tag{3.6.29}$$

$$W_{u/s} = \frac{-\Delta_f\, Z^2 - \Delta_u\, Z^2 + \Delta_u^2\, Z + 2\Delta_f \Delta_u\, Z + \Delta_f^2\, Z}{\Delta_f (\Delta_u^2 + \Delta_f \Delta_u)} \tag{3.6.30}$$

$$W_{f\,u/s} = \frac{\Delta_u\, Z^2 - 2\Delta_f \Delta_u\, Z - \Delta_u^2\, Z + \Delta_f (\Delta_u^2 + \Delta_f \Delta_u)}{\Delta_f (\Delta_u^2 + \Delta_f \Delta_u)} \tag{3.6.31}$$

Where Z as the distance from the far upstream node to the cell wall under consideration.

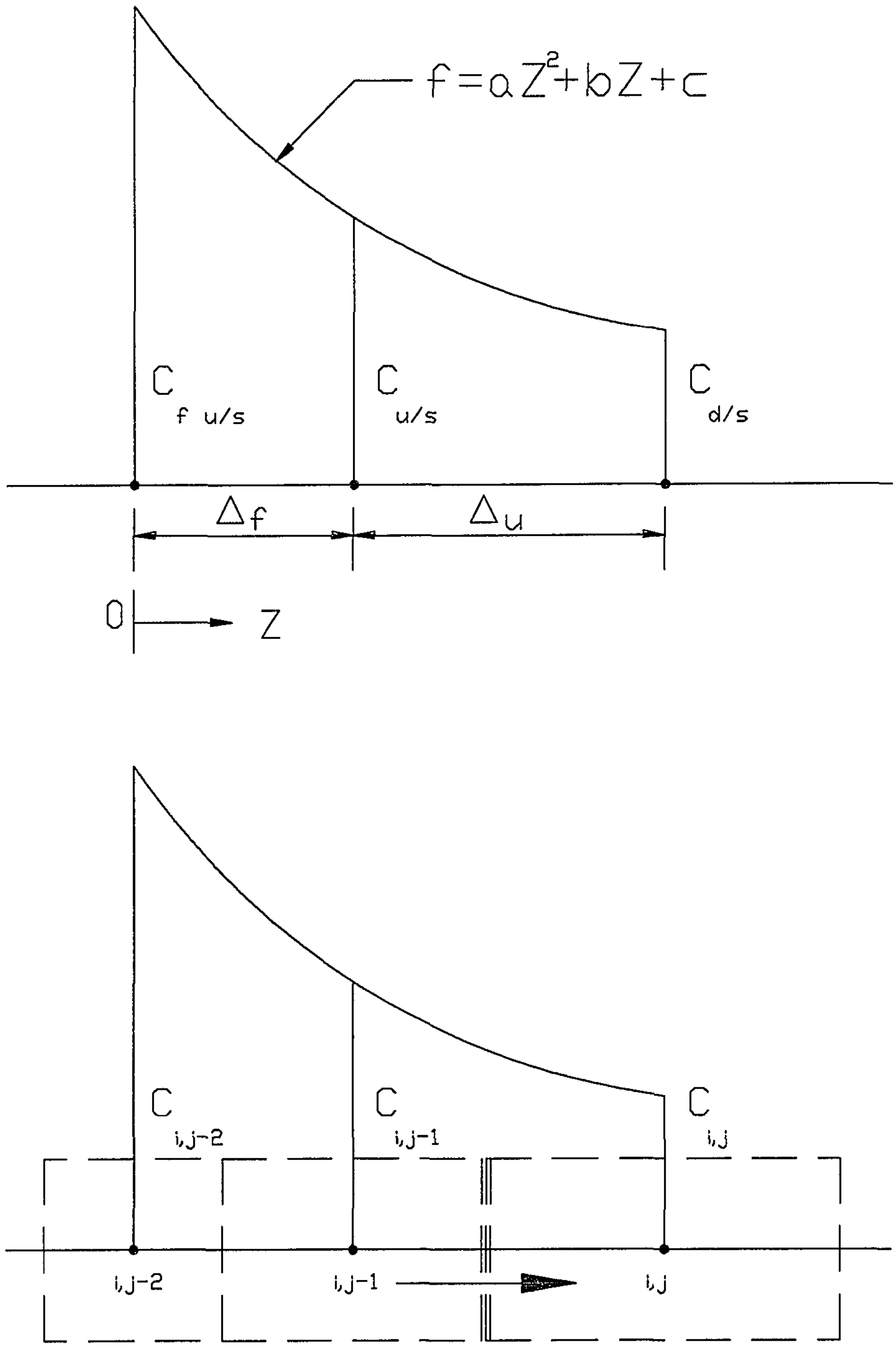


FIG. 3.7: DEFINITION SKETCH FOR DETERMINING CELL WALL CONCENTRATION USING QUADRATIC UPSTREAM INTERPOLATION

Depending on the flow direction, one can construct two distinct cases for each face of the cell. In all there would be eight cases. These cases are explained in detail in Appendix A2.

The dispersion component of the transport process in this scheme is the same as explained in Section 3.6.2. The finite difference equations for dispersive component is given in Eq. 3.6.6 through Eq. 3.6.9. The mass of the solute transported by way of advection is a product of groundwater flow and concentration entering the Cell (i,j) through each of the four faces. The flow terms are same as expressed in Eq. 3.6.19 through Eq. 3.6.22. The advection component using the quadratic upstream interpolation is expressed individually for each face of the aquifer cell.

Advective component in X direction, for mass entering the Cell (i,j) from left face

$$AD1 = T1(W_{10}C_{i,j}+W_{11}C_{i,j-1}+W_{12}C_{i,j-2}+W_{13}C_{i,j+1}+W_{14}C_{i,j+2}) \quad (3.6.32)$$

Advective component in X direction, for mass entering the Cell (i,j) from right face

$$AD3 = T3(W_{30}C_{i,j}+W_{31}C_{i,j-1}+W_{32}C_{i,j-2}+W_{33}C_{i,j+1}+W_{34}C_{i,j+2}) \quad (3.6.33)$$

Advective component in Y direction, for mass entering the Cell (i,j) from top face

$$AD2 = T2(W_{20}C_{i,j}+W_{21}C_{i-1,j}+W_{22}C_{i-2,j}+W_{23}C_{i+1,j}+W_{24}C_{i+2,j}) \quad (3.6.34)$$

Advective component in Y direction, for mass entering the Cell (i,j) from bottom face

$$AD4 = T4(W_{40}C_{i,j}+W_{41}C_{i-1,j}+W_{42}C_{i-2,j}+W_{43}C_{i+1,j}+W_{44}C_{i+2,j}) \quad (3.6.35)$$

where weights W_{mn}, m = 1, 2, 3 or 4, refers to left, top, right, or bottom face, respectively, and n = 0, 1, 2, 3, and 4, for terms in X direction these are refered to the nodes (i,j), (i,j-1), (i,j-2), (i,j+1), and (i,j+2), and for the terms in Y direction these are refered to nodes (i,j), (i-1,j), (i-2,j), (i+1,j), and (i+2,j). For example, weight W_{10} is defined as the weight associated with cell (i,j) for the mass entering the cell (i,j) from left face, similarly weight W_{23} is defined as weight associated with cell (i+1,j) for the mass entering the cell (i,j) from the top face.

Depending on the flow direction at the cell wall, only three weights associated with downstream, upstream, and far upstream are defined in the Eq. 3.6.32 through Eq. 3.6.35 (the weights are defined in Eq. 3.6.29 through Eq. 3.6.31). The remaining two weights are assigned a value zero as the case may be.

As in the case of groundwater flow component, the block centered finite difference formulation for dispersive component and quadratic upstream interpolation formulation for advective component for the governing advection-dispersion equation given in Eq. 3.6.1, follows from the application of continuity of mass: sum of all mass flow rates into and out of a Cell (i,j) that has sides Δx_j and Δy_i must equal rate of change of mass in the aquifer element.

$$
\begin{aligned}
& Dxx1\ (C_{i,j-1}^{n+1} - C_{i,j}^{n+1}) + Dxx3\ (C_{i,j+1}^{n+1} - C_{i,j}^{n+1}) + \\
& Dyy2\ (C_{i-1,j}^{n+1} - C_{i,j}^{n+1}) + Dyy4\ (C_{i+1,j}^{n+1} - C_{i,j}^{n+1}) + \\
& T1\ (W_{10}C_{i,j}^{n+1} + W_{11}C_{i,j-1}^{n+1} + W_{12}C_{i,j-2}^{n+1} + W_{13}C_{i,j+1}^{n+1} + W_{14}C_{i,j+2}^{n+1}) + \\
& T3\ (W_{30}C_{i,j}^{n+1} + W_{31}C_{i,j-1}^{n+1} + W_{12}C_{i,j-2}^{n+1} + W_{13}C_{i,j+1}^{n+1} + W_{14}C_{i,j+2}^{n+1}) + \\
& T2\ (W_{20}C_{i,j}^{n+1} + W_{21}C_{i-1,j}^{n+1} + W_{22}C_{i-2,j}^{n+1} + W_{23}C_{i+1,j}^{n+1} + W_{24}C_{i+2,j}^{n+1}) + \\
& T4\ (W_{40}C_{i,j}^{n+1} + W_{41}C_{i-1,j}^{n+1} + W_{42}C_{i-2,j}^{n+1} + W_{43}C_{i+1,j}^{n+1} + W_{44}C_{i+2,j}^{n+1}) - \\
& d_k(\phi\ b_{i,j}\Delta x_j\ \Delta y_i)\, C_{i,j}^{n+1} + C'_{i,j}Q'_{i,j} - Qw_{i,j}C_{i,j}^{n+1} \\
& \qquad = (\phi\ b_{i,j}\Delta x_j\ \Delta y_i)\left(\frac{C_{i,j}^{n+1} - C_{i,j}^{n}}{\Delta t}\right)
\end{aligned}
\tag{3.6.36}
$$

where ϕ is the aquifer porosity, W's are the weights associated as the case may be on the downstream, upstream and far upstream, d_k is the decay rate [1/T], Q_w is the groundwater pumping associated with the node (i,j), C' and Q' are the concentration and waste discharge rate of the external sources, n is the time step.

3.7 STOCHASTIC SPATIAL DISPERSIVITY FIELD

Like hydraulic conductivity, dispersivities are also functions of space and vary throughout the aquifer. The best localized values of these are determined in the field by conducting tracer tests, in which a dye is injected into the aquifer and its spread is measured in space. The procedure outlined under stochastic generation of hydrogeologic parameters (see Section 3.3) can be used to calculate multiple realizations of dispersivities. Provision is made in the computer program to compute this. However, it is felt there is no need to generate this stochastic field, because the stochastic conductivity field generated provides an indirect random field in computation of dispersion coefficient.

3.8 UNIT-CONCENTRATION RESPONSE MATRIX

The response of the system in terms of change in concentration at certain key locations (which are of critical interest in managing the system) due to unit-concentration injection rate at each potential injection well locations considered separately are recorded as unit-concentration response coefficients. Unit-concentration injection rate as defined by Gorelick and Remson (1982b) "can be any arbitrary but convenient groundwater solute source flux at a single location and which allows solutes to enter the aquifer for a specified period". These responses are assembled into a response matrix that is then included in the management model as a set of constraints together with the management and environmental constraints.

3.8.1 Potential Injection Well Location

As in unit-response matrix of groundwater flow component (discussed in Section 3.4.1), for generation of unit-concentration response matrix, it is necessary to identify all potential injection well locations. These potential injection wells may include all existing injection well locations together with a set of newly identified injection well locations. Along with identification and location of all injection wells, it is necessary to have injection rates defined at all these locations. This would allow the velocity field to be well defined, and therefore only the optimal concentration injection pattern is to be determined using the management model.

Stream reaches in an aquifer cell is treated in the model as a potential injection well location. The injection rate at stream cells (induced infiltration rates) either positive or negative is known or well defined from the management for water quantity.

3.8.2 Unit-Concentration Response Function, γ

In the governing advection-dispersion equation (Eq. 3.6.1), the dependent variable C(x,y,t), has a variable coefficient in velocity, U(x,y,t). Strictly speaking Eq. 3.6.1 is non-linear. In this research work a unique approach is used. When written in finite difference form the Eq. 3.6.1 is linear for each time step provided that the velocities are known. The groundwater velocity, U(x,y,t), is well defined within each time step. This allows the pde (Eq. 3.6.1) to be linear within that time step. Unit-concentration response function, γ , obtained by applying a unit-injection rate only in the first time-step and recording the changes in concentration over the entire simulation period is repeated for applying unit-injection rate in each of the subsequent time steps and recording the changes in concentrations over the entire simulation period. Compared to one simulation run in generating unit-response function in aquifer flow for each potential pumping well, here we have NT simulation runs (where NT is the number of time steps) for each potential injection well. Although, this is computationally intensive, it gives us the advantage to apply superposition, as if treating the governing pde as linear.

3.8.3 Superposition Using Unit-Concentration Response Function

The concentration at any point k (for example pumping well), within the aquifer resulting from NRW injection wells, for KT time periods, and for any realization KR, is given by

$$C(k,KT) = C_o - \sum_{jrw=1}^{NRW} \sum_{it=1}^{KT} \gamma(k,jrw,KT,it,KR)\, W_L(jrw,it) \quad (3.8.1)$$

where, C(k,KT) = concentration at any point k at time step KT, W_L(jrw,it) = wastewater

load of solute injected at well jrw during itth period, γ (k,jrw,KT,it,KR) = system unit-source concentration response coefficients in the KT time-step at any point k as a result of unit injection rate at injection well jrw for unit injection in the itth time step in realization KR.

3.9 SOLUTE TRANSPORT COMPONENT OF STREAMS

In order to consider solute transport in streams, two basic assumptions are made. Firstly, in streams, advection is a dominant way of solute transport, owing largely to the magnitude of the velocities associated in the flow. Secondly, a river or stream is assumed to be homogeneous with respect to water quality variables across the river (laterally) and depth (vertically). With these two assumptions, the one-dimensional basic partial differential equation for an advective nondispersive stream with a source term and first order reaction is given by:

$$\frac{\partial (C_R A)}{\partial t} = -\frac{\partial (C_R Q)}{\partial x} + q_{WD} C_R^{\prime} - d_{ks} C_R A \qquad (3.9.1)$$

where, C_R = concentration in the stream, Q = stream flow, d_{ks} = first order reaction coefficient, q_{WD} = effluent waste discharge into the stream per unit length, $C_R^{\prime}$ = effluent concentration, and A = flow area. The sketch for the control volume approach is shown in Fig. 3.8.

As in the groundwater solute transport component, the pde described in Eq. 3.9.1 has two state variables: the stream concentration, $C_R(x,t)$, and stream flow, $Q(x,t)$. The actual streamflows as obtained from the optimization of flow quantities is substituted in here. The pde described in Eq. 3.9.1 is solved for the unknown stream concentration.

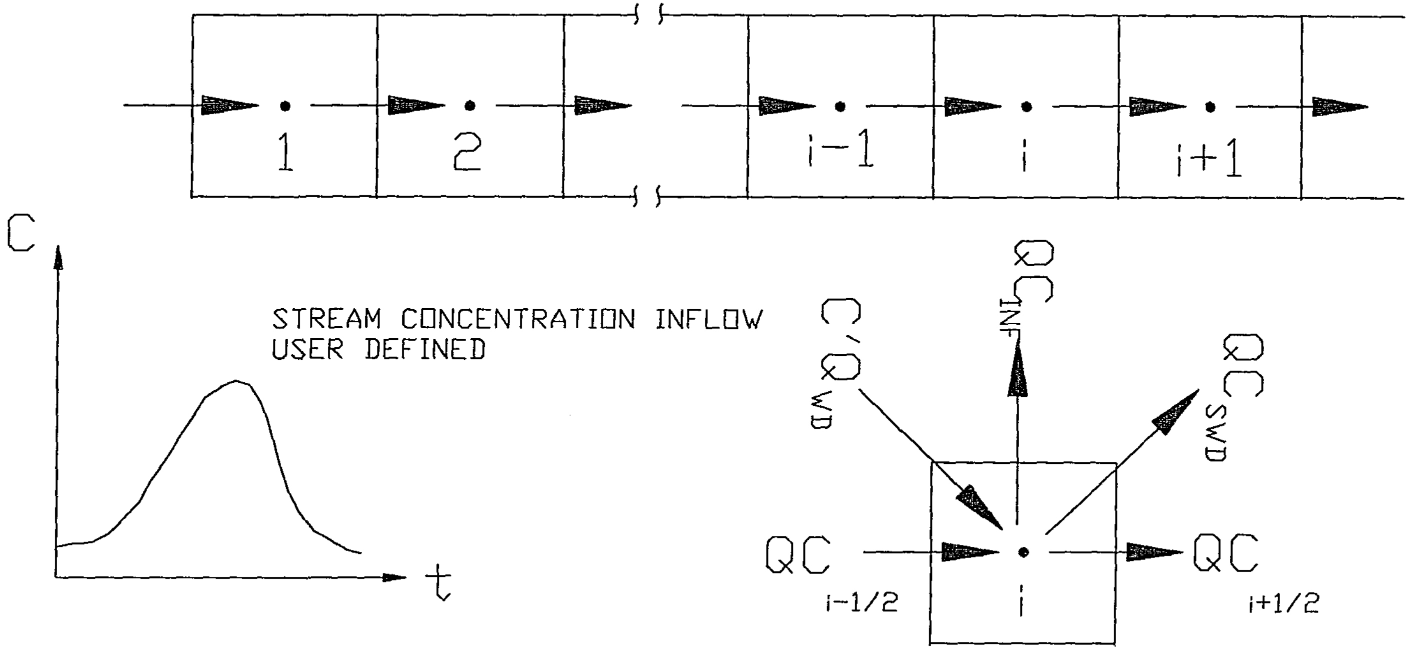


FIG. 3.8: CELL NUMBERING NOTATION FOR ONE-DIMENSIONAL SOLUTE TRANSPORT IN STREAMS

3.9.1 Finite Difference Equation

Fig. 3.8 shows the cell numbering notation used in the block centered finite difference grid of the one-dimensional mass transport in streams for any time increment, Δt, the finite difference form of Eq. 3.9.1 is expressed as

$$\frac{(C_R Q)^n_{i-\frac{1}{2}} + (C_R Q)^{n+1}_{i-\frac{1}{2}}}{2} - \frac{(C_R Q)^n_{i+\frac{1}{2}} + (C_R Q)^{n+1}_{i+\frac{1}{2}}}{2} + \frac{(C'_R Q_{WD})^n_i + (C'_R Q_{WD})^{n+1}_i}{2} - \frac{(d_{ks} C_R S)^n_i + (d_{ks} C_R S)^{n+1}_i}{2} - \frac{(C_R Q_{SWD})^n_i + (C_R Q_{SWD})^{n+1}_i}{2} \pm \frac{(C_R Q_{INF})^n_i + (C_R Q_{INF})^{n+1}_i}{2} = \frac{(C_R S)^{n+1}_i - (C_R S)^n_i}{\Delta t} \tag{3.9.2}$$

where, n refers to the time step, $C_{i-1/2}$ refers to concentration on the upstream or left face, similarly $C_{i+1/2}$ refers to concentration on the downstream face of the reach, S is the storage of the reach defined by Eq. 3.5.13, $Q_{WD} = \Delta x_i\, q_{WD}$ = the effluent waste discharge into the stream reach, $Q_{i-1/2}$ is the upstream inflow to the reach defined by Eq. 3.5.14, and $Q_{i+1/2}$ is the downstream outflow given by Eq. 3.5.15.

In modeling stream transport upstream differencing scheme is used, by defining $C_{i-1/2} = C_{i-1}$, and $C_{i+1/2} = C_i$. For the first reach the upstream inflow concentration rate is user specified.

3.10 COMPREHENSIVE CONJUNCTIVE-USE MANAGEMENT MODEL

The various components detailed above have been integrated here to seek the optimal solution for the management problem. A typical management model consists of an objective function subjected to a set of constraints. In this research work we are

concerned with maximizing the surface water withdrawal together with pumpage of groundwater. At the same time we are interested in maximizing the waste input concentration into surface water and groundwater. The simultaneous optimization of flow and quality aspects lead to a highly nonlinear, possibly nonconvex optimization problem. In order to facilitate the solution of this complex problem, at first the stochastic management of water quantity aspects described by the groundwater flow component (see Section 3.2), and surface water flow component (see Section 3.5) is formulated and solved. In the next step, the system response thus obtained, is used in framing the stochastic management model of water quality aspects described by the solute transport component of groundwater (see Section 3.6), and surface water (see Section 3.9). The optimal solution for the water quality aspects are then obtained by solving the management problem formulated.

3.10.1 Management Model for the Water Quantity Aspects

In the simulation-optimization procedure developed here, the aquifer response due to unit-excitation is known by simulation at all points of interest. As mentioned in Section 3.4, the actual drawdowns at all points of interest can be easily obtained by the principle of superposition (Eq. 3.4.2), if the actual excitation pattern is known. In the developed management model we seek an optimal excitation pattern at all potential wells, and optimal withdrawal from surface water, subjected to a set of system, management, and environmental constraints.

3.10.1.1 Objective Function - Water Quantity

The objective function to find optimal pumping from all the potential pumping wells, and optimal surface water diversions is expressed as

$$Max\ Z = \sum_{jw=1}^{NW} \sum_{it=1}^{NT} Q_w(jw,it) + \sum_{js=1}^{NSWD} \sum_{it=1}^{NT} Q_{SWD}(js,it) \qquad (3.10.1)$$

where, $Q_w(jw,it)$ = well pumpage from jw[th] well during the it[th] period, and $Q_{SWD}(js,it)$ = surface water diversion from js[th] reach during the it[th] period, NT is the total number of time steps, NW is the number of pumping wells, and NSWD is the number of surface water diversion locations along the stream. In the model Q_w's (total of NW*NT) and Q_{SWD}'s (total of NSWD*NT) form a set of decision variables. This is subject to the system, management, and environmental constraints, these are discussed below:

3.10.1.2 System Constraints - Groundwater Surface Water Interaction

The induced infiltration, Q_{INF}, is an implicit function of river head, hr, and aquifer head in the river cell, h (ref Section 3.5.3). In the management model these form as a set of system constraints which are non-linear equality constraints. The implicit equation for the reach i, time step KT, and realization KR is expressed as

$$\frac{P'}{m} As_i \{hr_i^{KT} - (h_o - \left[\sum_{it=1}^{KT} \sum_{jw=1}^{NW} \beta(i,jw,KT-it+1,KR)\ Q_w(jw,it)\right] + \left[\sum_{it=1}^{KT} \sum_{ir=1}^{NR} \beta(i,ir,KT-it+1,KR) Q_{INF}(ir,it)\right])\} - Q_{INF}^{KT} = 0 \qquad (3.10.2)$$

where, river head $hr = y + hr_b$, and hr_b is the river bed elevation in the reach, and y is the

stream flow depth, P' is the stream bed permeability, m is the stream bed thickness, A_s is the surface area of the stream in the cell, and h_0 is the initial piezometric surface.

As can be seen in Eq. 3.10.2, Q_{INF} is a system variable and can be fully expressed by aquifer head and river head. Here, Q_{INF}'s (total of NRIVER*NT) are treated as decision variables for convenience in setting up the stream mass balance equations. Eq. 3.10.2 is repeated for all the river reaches (NRIVER reaches), and for all the time steps.

3.10.1.3 System Constraints - Stream Mass Balance Equations

Unsteady flow equations of the streams are modeled as system constraints. These are non-linear equality constraints, described by the Eq. 3.5.12, and the same is expressed below for clarity.:

$$\frac{S_i^{n+1} - S_i^n}{\Delta t} = \frac{Q^n_{i-\frac{1}{2}} + Q^{n+1}_{i-\frac{1}{2}}}{2} - \frac{Q^n_{i+\frac{1}{2}} + Q^{n+1}_{i+\frac{1}{2}}}{2} - \frac{Q^n_{SWD_i} + Q^{n+1}_{SWD_i}}{2} \pm \frac{Q^n_{INF_i} + Q^{n+1}_{INF_i}}{2} + \frac{Q^n_{WD_i} + Q^{n+1}_{WD_i}}{2} \qquad (3.10.3)$$

In Eq. 3.10.3 the waste discharge input to the stream Q_{WD} is a known quantity, and as mentioned earlier Q_{SWD} and Q_{INF} are a set of decision variables. The stream depth in the reach centroid is also grouped into the set of decision variables (total of NRIVER*NT). In Eq. 3.10.3 storage of a reach is expressed in terms of flow depth (Eq. 3.5.13), and inflow and outflow of a reach in terms of flow depth (Eq. 3.5.14 and Eq. 3.5.15). The upstream boundary condition in terms of either a user specified or synthetic hydrograph generated is incorporated while writing the mass balance equation for the most upstream reach.

Eq. 3.10.3 is repeated for all reaches (NRIVER), and for (NT - 1) time steps.

3.10.1.4 System Constraints - Stream Initial Condition

Uniform flow is assumed with no surface water diversions in the first time step. These are linear equality constraints, and in the model the stream initial condition is expressed as

$$Q_i^1 = Q_{i+1}^1 \tag{3.10.4}$$

where, Q_i^1 is the discharge in the reach section i, in time step 1. Eq. 3.10.4 is repeated for all the river sections (2,3,... to NRIVER+1). In the model the discharges are expressed in terms of flow depth described by the Eq. 3.5.15.

3.10.1.5 Management Constraints - Aquifer Drawdowns

The maximum permissible drawdown at location k in any time period KT, $s^*(k,KT)$, to prevent the rate of depletion, or to prevent undesirable effects such as salt water intrusion, land subsidence, or acceleration of contaminant movement, serves as one of the management constraints for the aquifer flow system. This is a linear inequality constraint, and in the model it is expressed as

$$\sum_{jw=1}^{NWR} \sum_{it=1}^{KT} \beta(k,jw,KT-it+1,KR)\ Q_w(jw,it) \leq s^*(k,KT) \tag{3.10.5}$$

This constraint is repeated for all points of interest, k = 1,2,..jj, NWR = number of potential pumping wells plus river reaches, and β represents the response function

obtained for realization KR of hydraulic conductivity and storativity and the constraint is repeated for all realizations and for all time steps. On the left hand side of the Eq. 3.10.5, response of injection wells are also added expressing in a similar fashion.

3.10.1.6 Management Constraints - Stream Depth

The maintenance of minimum stream flow depth in any time step KT, $yr^*(KT)$, to meet downstream water rights, or to help preserve the aquatic life, serves as the management constraint for surface water. The constraints are set up for the last reach, as this is the most critical one. This is a non-linear inequality constraint and expressed as

$$Y_R(NR, KT) \geq Y_R^*(KT) \qquad (3.10.6)$$

This constraint is written only for the last reach, NR, and for all time periods KT = 1,2,...,NT.

3.10.1.7 Management Constraints - Water Demand

In the development of water resources, one of the primary objectives is to satisfy the water demands (for meeting domestic and industrial needs) of a region. The water demands may be met by supplies from pumping wells which tap an aquifer and/or by diversion from a stream. The total quantity pumped from the aquifer is restricted by well capacities and allowable/or permissible drawdowns in the aquifer. The total amount of water that can be removed from the stream by direct diversion or by induced infiltration is limited by the necessity of maintaining a minimum streamflow or minimum

stream depth downstream of the diversion point. This is classed as a management constraint which is a linear inequality constraint, and is expressed in the model as

$$\sum_{jw=1}^{NW} Q_w(jw,it) \ + \sum_{js=1}^{NSWD} Q_{SWD}(js,it) \ \geq \ D^*(it) \tag{3.10.7}$$

This constraint is repeated for all time periods it = 1,2,...,NT and $D^*(it)$ = water demand during itth period. The constraint expressed in Eq. 3.10.7, satisfies water demand by pumping water from wells, and by surface water diversions. If the management involves so as to meet a portion of the water demand, $D_w^*(it)$, by only groundwater wells, this type of constraint is expressed in the model as

$$\sum_{jw=1}^{NW} Q_w(jw,it) \geq D_w^*(it) \tag{3.10.8}$$

This constraint is repeated for all the time steps it = 1,2,...NT, where NT is the total number of time steps.

3.10.1.8 Pumping Well Capacity Constraints

Depending on the type and number of pumps installed at a pumping well location, the combined maximum pumping capacity of each individual well varies. This cap on the pumping capacity is a linear inequality constraint, and is expressed in the model as

$$Q_w(jw,it) \ \leq \ Q_w^{\max}(jw,it) \tag{3.10.9}$$

For all wells jw = 1,2,...,NW and during all time periods it = 1,2,...,NT, this constraint is repeated.

3.10.1.9 Surface Water Diversion Capacity Constraints

On similar lines to pumping well capacity constraints, a cap for surface water diversion in the form of a linear inequality constraint is expressed in the model as

$$Q_{SWD}(js,it) \leq Q_{SWD}^{max}(js,it) \qquad (3.10.10)$$

For all diversion points js = 1,2,...,NSWD and during all time periods it = 1,2,...,NT, this constraint is repeated.

3.10.1.10 Optimization Routine for Water Quantity

The control parameters for the management model so framed is given in Table 3.10.1.

Table 3.10.1

Control Parameters for Optimization of Water Quantity

Description	Name	Value
Total number of decision variables	NDV	(NW + 2*NR + NSWD)*NT
Total number of constraints (if NR > 0)	NTCE	NR*2*NT + 3*NT + (NW+NP)*NOR*NT + NSWD*NT + NSWD
Total number of constraints (if NR = 0)	NTCE	(NW+NP)*NOR*NT + NW*NT + NT
Number of non-linear equality constraints	NLEQ	2*NR*(NT-1)
Number of non-linear inequality constraints	NLIEQ	0
Number of linear equality constraints	LEQ	2*NR + NSWD
Number of linear inequality constraints	LIEQ	(NW+NP)*NOR*NT + (NW*NT) + NSWD*NT + 3*NT

The optimization routine used in this research is NEWSUMT-A (stands for new algorithm for a sequence of unconstrained minimization technique) which can handle non-linear optimization with equality and inequality constraints, developed by Thareja and Haftka (1985). The details of the optimization routine can be found in their report.

In brief NEWSUMT-A is a general purpose optimizer written in FORTRAN subroutine form that can be used for solving a wide variety of numerical optimization problems. NEWSUMT-A uses an extended interior penalty for inequality constraints and an exterior penalty for equality constraints and the direction of the move is found by Newton's method with approximate second derivatives. The computational procedure adopted in the optimizer is briefly discussed in Appendix A4.

After seeking the optimal solution for the above management problem, the simulation model determines the system response of the combined system defined by the piezometric heads in the aquifer for the optimal well pumpages with induced infiltration from surface water by executing the simulation program for each realization.

3.10.2 Management Model for Water Quality Aspects

Once the piezometric heads are obtained throughout the aquifer, we proceed with the simulation-optimization procedure for water quality. From the numerical simulation model for the solute transport unit-source concentration response matrix is obtained. This response matrix is then used in the optimization model as constraints for the management of water quality aspects.

As mentioned in Section 3.8, the actual concentrations at all points of interest (such as pumping wells) can be determined by principle of superposition (Eq.

3.8.1), if the actual concentration injection pattern at each of the potential injection well is known. In the management model we seek optimal injection concentration pattern at all potential injection wells, and optimal disposal concentration pattern into surface water, subjected to a set of system and management constraints.

3.10.2.1 Objective Function - Water Quality

The objective function to find optimal concentration injection in all potential injection wells, and optimal concentration disposal into surface water is expressed in the model as

$$Max\ Z = \sum_{jrw=1}^{NRW} \sum_{it=1}^{NT} C_w^{/}(jrw,it) + \sum_{jrs=1}^{NDSW} \sum_{it=1}^{NT} C_R^{/}(jrs,it) \qquad (3.10.11)$$

where, $C_w^{/}$ (jrw,it) = concentration injected into the jrwth well during the itth period, $C_R^{/}$ (jrs,it) = concentration disposed into the river at jrsth reach during the itth period. NRW is the number of recharge or injection wells, NDSW is the number of reaches where waste disposal of concentration is expected. In the model $C_w^{/}$ (total of NRW*NT) and $C_R^{/}$ (total of NDSW*NT) form a set of decision variables. This is subject to a set of system, management and environmental constraints, and these are discussed individually below.

3.10.2.2 System Constraints - Stream Mass Balance Equation

The unsteady transport equation for streams are modeled as system constraints. These are linear equality constraints, described by the Eq. 3.9.2, and the same is expressed below:

$$\frac{(C_RQ)^{n}_{i-\frac{1}{2}} + (C_RQ)^{n+1}_{i-\frac{1}{2}}}{2} - \frac{(C_RQ)^{n}_{i+\frac{1}{2}} + (C_RQ)^{n+1}_{i+\frac{1}{2}}}{2} + \frac{(C'_RQ_{WD})^{n}_{i} + (C'_RQ_{WD})^{n+1}_{i}}{2} - \frac{(d_{ks}C_RS)^{n}_{i} + (d_{ks}C_RS)^{n+1}_{i}}{2} - \frac{(C_RQ_{SWD})^{n}_{i} + (C_RQ_{SWD})^{n+1}_{i}}{2} \pm \frac{(C_RQ_{INF})^{n}_{i} + (C_RQ_{INF})^{n+1}_{i}}{2} = \frac{(C_RS)^{n+1}_{i} - (C_RS)^{n}_{i}}{\Delta t} \tag{3.10.12}$$

where, n refers to the time step, $C_{i-1/2}$ refers to concentration on the upstream or left face, similarly $C_{i+1/2}$ refers to concentration on the downstream face of the reach. Storage S, upstream inflow, $Q_{i-1/2}$, and downstream outflow, $Q_{i+1/2}$, of a reach together with surface water diversion rate, Q_{SWD}, and waste discharge disposal rate, Q_{WD}, are known quantity from the optimization of water quantity. The only variable stream concentration defined at the centroid of a reach is unknown, which is grouped into the set of decision variables.

In modeling the surface water groundwater interaction for water quality, any loss of surface water by way of induced infiltration carries the concentration associated in that reach into the aquifer. Here, it is assumed that pollutant input from the aquifer to the stream has negligible effect on streamflow quality compared to direct waste disposal into the stream. This assumption is done mainly due to order of magnitude difference between streamflow and induced infiltration rate recharging the stream, any groundwater concentration associated with the induced infiltrtion rate would make significantly less impact to the streamflow concentrtion.

3.10.2.3 System Constraints - Stream Initial Condition

As in surface water flow component, uniform flow is assumed with no waste disposal discharge in the first time step. These are linear equality constraints and in the model initial condition of the stream is expressed as

$$C_R(i,1) = C_R(i+1,1) \qquad (3.10.13)$$

where, $C_R(i,1)$ refers to concentration in the reach i in time step 1. Eq. 3.10.13 is repeated for all reaches.

3.10.2.4 Management Constraints - Aquifer Concentrations

The maximum permissible concentration at any location k during any time period KT, C_w^* (k,KT), is not to be exceeded to protect / prevent pollution of aquifer in the vicinity of pumping wells. This is modeled as a linear inequality management constraint and expressed in the model as

$$C_o(k) - \sum_{jrw=1}^{NRWR} \sum_{it=1}^{KT} \gamma(k,jrw,KT,it,KR)\, W_L(jrw,it) \le C_w^*(k,KT) \qquad (3.10.14)$$

This constraint is repeated for all points of interest, k = 1,2,..jj, NRWR = number of potential injection wells plus river reaches, and γ represents the unit-source concentration response function obtained for realization KR of hydraulic conductivity and storativity and the constraint is repeated for all realizations.

3.10.2.5 Management Constraint - River Water Quality

The waste disposal of concentration into surface water needs to be contained so as not to pollute the stream than a maximum permissible concentration, C_R^* (it), to help protect aquatic life, or to maintain downstream water quality. The constraints are set up for the last reach, as this is the most critical one. This is a linear inequality constraint and expressed in the model as

$$C_R(NR, it) \leq C_R^*(it) \tag{3.10.15}$$

where, C_R(NR,it) = concentration of river water in the last reach, NR, during the time period it and C_R^* (it) = maximum permissible concentration in the river during the time period it. This constraint is repeated for all the time steps.

3.10.2.6 Management Constraint - Waste Load Disposal Demand

The determination of optimal concentration injection or disposal pattern needs to meet the waste load generated in the region. This is set up as a management constraint which is linear and expressed as

$$\sum_{jrw=1}^{NRW} Q_w'(jrw, it)\ C_w'(jrw, it)\ + \sum_{jrs=1}^{NDSW} Q_d'(jrs, it)\ C_R'(jrs, it) \geq W_L^*(it) \tag{3.10.16}$$

This constraint is repeated for all time steps it = 1,2,...,NT and W_L^*(it) = waste load demand during the itth period. The constraint expressed by Eq. 3.10.16 satisfies waste load demand by injection at recharge wells, and disposal at surface water. If the

management involves so as to meet portion of waste load, WL^*_{INJ}, to be met only by injection into aquifer, such constraints are expressed in the model as

$$\sum_{jrw=1}^{NRW} Q'_w(jrw,it)\ C'_w(jrw,it) \geq WL^*_{INJ}(it) \qquad (3.10.17)$$

3.2.10.7 Injection Well Capacity Constraints

Depending on the design of a recharge well and type and number of injection pumps installed at a injection well site the maximum concentration injection capacity of each injection well varies. This cap on the injection capacity is set up as a linear inequality constraint in the model and is expressed as

$$Q'_w(jrw,it)\ C'_w(jrw,it) \leq Q'_w(jrw,it)\ C^{\max}_w(jrw,it) \qquad (3.10.18)$$

This constraint is repeated for all injection wells, NRW, and for all time steps, NT. As can be seen in the Eq. 3.10.18 the waste load discharge rate, Q'_w (jrw,it), is a known quantity and appears on both sides of the equation. In effect the constraint (Eq. 3.10.18) is set on the maximum permissible concentration injection.

3.10.2.8 Surface Water Disposal Capacity Constraints

On similar lines to injection well capacity, a cap for surface water disposal capacity is set up as linear inequality constraints and is expressed in the model as

$$Q'_R(jrs,it)\ C'_R(jrs,it) \leq Q'_R(jrs,it)\ C^{\max}_R(jrs,it) \qquad (3.10.19)$$

where, $C^{\max}_R$ (jrs,it) = maximum concentration disposal in a river reach. This constraint

is repeated for all surface water disposal sites, NDSW, and for all time steps, NT.

3.10.2.9 Optimization Routine for Water Quality

The control parameters for the management model for water quality so framed is given in Table 3.10.2.

Table 3.10.2

Control Parameters for Optimization of Water Quality

Description	Name	Value
Total number of decision variables	NDV	(NRW + NR + NDSW)*NT
Total number of constraints (if NR > 0)	NTCE	NR*NT + 3*NT + (NW+NP)*NOR*NT + (NRW+NDSW)*NT + NDSW
Total number of constraints (if NR = 0)	NTCE	(NW+NP)*NOR*NT + NRW*NT + NT
Number of non-linear equality constraints	NLEQ	0
Number of non-linear inequality constraints	NLIEQ	0
Number of linear equality constraints	LEQ	NR*NT + NDSW
Number of linear inequality constraints	LIEQ	(NW+NP)*NOR*NT + (NRW + NDSW)*NT + 3*NT

The optimal concentration injection pattern with optimal concentration disposal into surface water is determined by calling NEWSUMT-A optimization routine. After seeking the optimal concentration injection pattern, the transport simulation model developed determines the system response of the combined system defined by aquifer concentrations.

3.10.3 Optimization Using Linear Programming

The non-linear optimization routine NEWSUMT-A used in this research work handles both linear and non-linear equality and inequality constraints efficiently. The non-linearity in the conjunctive-use management model discussed in Section 3.10.1, arises soley due to the governing system equations for stream mass balance and groundwater surface water interaction, which are non-linear equality constraints.

For aquifer management of flow and transport without streams the management model is described by a linear objective function subjected to a set of linear inequality constraints. Only for this case, wherein all the constraints are linear functions of decision variables, in the developed management model, the user has an option to use either non-linear optimization routine, NEWSUMT-A, or linear programming optimization routine, SIMPLEX. The SIMPLEX routine is a standard FORTRAN subroutine from the book titled "Numerical Recipes: The Art of Scientific Computing", by Press et al. (1992). As shown later in Section 4.6 under management model verification the solution obtained by NEWSUMT-A and SIMPLEX are in close agreement for an aquifer management problem.

4. MODEL VERIFICATION

An important step in the model development process is to verify how accurately the numerical results obtained represent the behaviour of the actual physical system. The methods available to verify the accuracy of the model are:

1. By applying the model developed to simulate the real physical system for which exhaustive field measurements, field observations, and in general all input data and output information are available. By performing such a simulation it can be easily verified how closely the model represents the actual behaviour of the system.

   During this research work no field research experiments were undertaken to collect all the information required for the model verification. Further, every attempt was made to collect the case studies published of the real physical systems. For the comprehensive conjunctive-use model developed here, the input data required to simulate a real system is exhaustive. None of the case studies reported gave adequate information with respect to input and output, as the case studies reviewed in essence dealt with much simpler physical systems than for the one developed here.

2. By comparing the model results to analytical solutions. In general analytical solutions are available only for a few simplified cases such as

homogeneous, isotropic, infinite areal extent with well defined initial and boundary conditions, although in reality such a physical system does not exist. However, these analytical solutions serves as a testing ground for the model developed. As discussed later in this section, the numerical solutions of the model are compared with available analytical solutions.

3. By comparing the results of the flow and transport component with the solutions of the available generic programs independently. Although, the available generic programs do not account for all the complexities and features built in this research work, as discussed later the comparison is made in a limited way as to what the generic programs can simulate.

4. By comparing the model solutions with published results (those published in either standard reference books or in technical journals are used). For instance, the results of the two-dimensional transport simulation block is compared with the method of characteristics solution reported in the USGS technical publication (Konikow and Bredehoeft, 1978). In general it was found that the models reported in the peer technical literature did not include all the needed input and output information necessary for model verification. Attempts to obtain all the missing information directly from the lead author failed, either due to published results were old and no back-up information available with them or the author was not available. Therefore, only a limited number of comparisons were made.

5. By introducing internal diagnostic checks in the model. Model components included in this research work has a built in internal diagnostic checks to

remove the possibility of any programming bugs. In the flow and transport model these internal diagnostic checks can be identified as:

a. Water balance and mass balance in the system. This is an internal running check for all the time steps.

b. Sum of changes in piezometric heads / concentration during each iteration over the entire model simulated should converge to an acceptable user specified tolerance. This is also an internal running check for all the time steps. This type of check works well with aquifer problems concerning regional analysis.

Also several external diagnostic checks were performed, such as the capability of the model to produce axially symmetric results under axially symmetric input data.

These internal and external diagnostic checks ensure to a great extent the accuracy of the model developed. Where verifications of the model using the standard methods discussed above are not possible, only these internal and external diagnostic checks serve to verify the model. These are also discussed later.

All the verification methods discussed above have their own limitations. A best effort is made in verifying the model results with at least one of the available methods. Due to scarcity and accuracy of all the input data required for the model, verification of all the model components developed together was not possible. Verification of the individual components developed are discussed below.

4.1 VERIFICATION OF THE GROUNDWATER FLOW COMPONENT

In verifying the groundwater flow component several tests were conducted. These tests are discussed individually below.

4.1.1 Check for Mass Balance

This is an internal running check for all the time steps. Mass balance is defined in the computer model as cumulative net sum of all external inflows and outflows should equal change in volume of water in storage. The check for mass balance is printed in the model output for every time step, and the sample of the same obtained in the 24^{th} time step for the model application problem considered in Section 5.1 is reflected in Table 4.1.1. The mass balance error of 0.04% is acceptable because of large pumping encountered.

4.1.2 Check for Symmetric Distribution of Flows

A homogeneous, isotropic aquifer with symmetrical constant head boundary conditions (constant head = 0 m on all four sides) is considered. The system is initially at rest (initial piezometric surface = 0 m throughout) and is subjected to a constant pumping of 20000 m^3/d from a symmetrically placed well in the center of the aquifer. The size of the aquifer is 9300 m x 9300 m, thickness = 40 m, constant permeability in the X and Y direction equal to 100 m/d, and the confined aquifer storage coefficient = 0.001. For a hypothetical problem the isopiestic lines of equal drawdown is shown in Fig. 4.1, which verifies the model behaviour for symmetric flow distribution.

Table 4.1.1

Check for Mass Balance - Flow Component

Storage Increase	81.93 m^3
Storage Decrease	-2074.70 m^3
TOTAL STORAGE CHANGE (Increase - Decrease)	-1992.77 m^3
Amount of Recharge from Boundary	10354829.00 m^3
Amount Discharged to Boundary	-292757.81 m^3
TOTAL (Recharge - Discharge) FROM BOUNDARY	10062071.00 m^3
Cumulative Leakage	1804582.38 m^3
Permanent Pumping Through Wells	0.0 m^3
Total Pumpage from Start	-37270280.00 m^3
Permanent Recharge Through Wells	0.0 m^3
Total Injection from Start	25400628.00 m^3
CUMULATIVE NET (Pumpage - Injection) OUTFLOW	-11869652.00 m^3
NET INFLOW (from Boundary + Storage Release + Leakage)	11868646.00 m^3
MASS BALANCE ERROR	**-0.04206%**

4.1.3 Comparison of the Model Results with Analytical Solution

The analytical solution for aquifer drawdowns for an unsteady, radial flow situation in a infinite, homogeneous, isotropic, non-leaky, confined aquifer with a single pumping well fully penetrated, and for constant discharge conditions is given by

$$s(r,t) = \frac{Q}{4\pi T} W(u), \quad u = \frac{r^2 S}{4Tt} \tag{4.1.1}$$

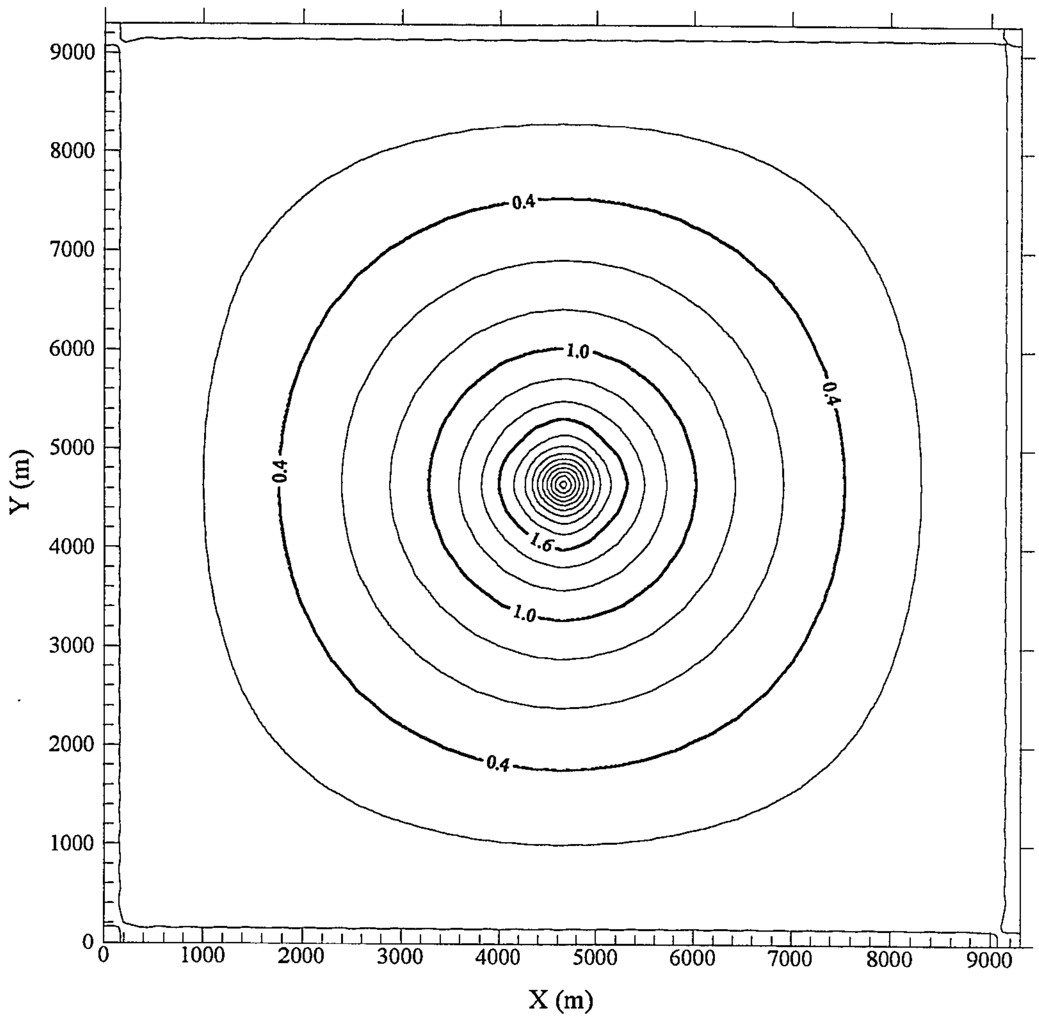


FIG 4.1: SYMMETRIC DISTRIBUTION OF DRAWDOWNS (m)

where r is the distance from the pumping well at any time t after the pumping has started, T = transmissivity, S = storage coefficient, and Q = constant well discharge.

An infinite aquifer was computer simulated by making the number of model rows and columns sufficiently large such that the piezometric heads at points of interest were not affected by the presence of the boundary edges of the model. Further, the assumption made here that the aquifer is of infinite areal extent, introduces no significant error in practical applications, although such an aquifer does not exist. This statement is valid as long as the cone of depression has not reached any aquifer boundary (ref: Bear (1979), pp 324).

The input to the computer model is tabulated below:

Aquifer Transmissivity, T	= 1000 m^2/d,
Storage Coefficient, S	= 1.003 x 10^{-2},
Grid Spacing $\Delta x = \Delta y$	= 300 m constant,
Density of Grid NROW = NCOL	= 31,
Time Step, Δt	: 0.5 d
	: 1.0 d
	: 5.0 d
	: 10. d
Constant well discharge, Q	= 3500 m^3/d
Pumping Well Location (i,j)	= (16,16)
Distance to observation point	= 300 m
Initial Piezometric Head, H_o	= 0.0 m throughout,

Barrier boundary condition on all four sides.

A time-drawdown graph in Fig. 4.2 illustrates the sensitivity of the computer simulated drawdowns for analytical solution as a result of varying the size of the discrete time increment Δt. The comparison in Fig. 4.2 reveals that at earlier time steps the discrepancy between the analytical solution and the model results decreased as Δt is reduced. However, for later time steps irrespective of discrete time increment, the difference between analytical and computer results are insignificant.

4.1.4 Comparison of the Model Results with PLASM

PLASM is a generic aquifer simulation model developed by Prickett and Lonnquist (1971). Fig. 4.3 shows the finite difference grid configuration used in comparing the numerical model (flow component) with PLASM. The considered aquifer is an example of the actual use of various features built into the model. The computer input data is summarized below:

Aquifer Transmissivity, T	= 600 m^2/d,
Storage Coefficient, S	= 0.0005,
Permeability of the Leaky bed	= 3.1253e-8 m/d
Thickness of the Leaky bed	= 1.0 m
Grid Spacing (ref: Fig 4.3)	= Variable,
Density of Grid NROW = NCOL	= 20,
Time Step, Δt	= 182.625 d
Number of Pumping Wells	= 7,
Initial Piezometric Head, H_o	= 0.0 m throughout,

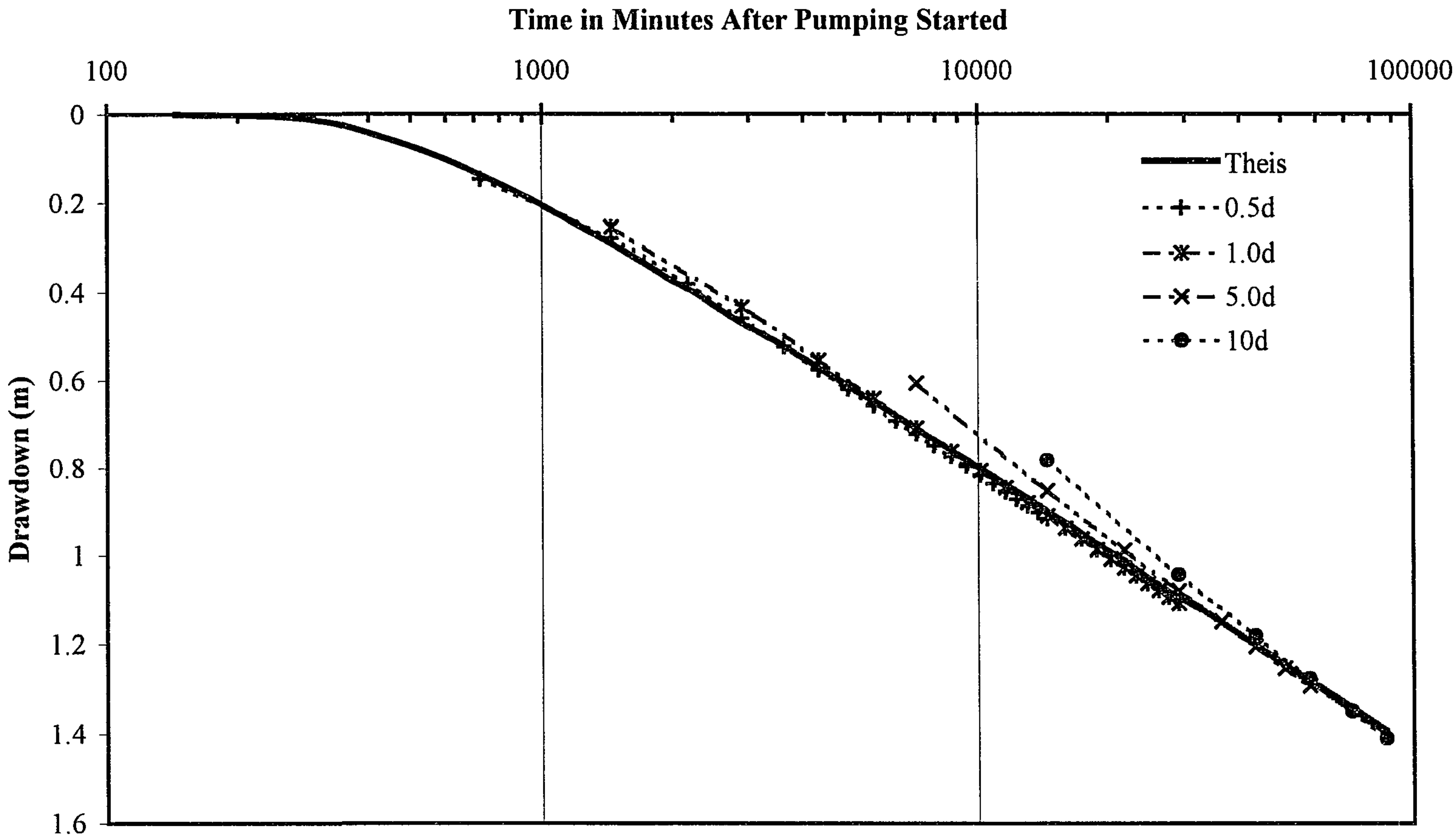


FIG 4.2: COMPARISON OF NUMERICAL MODEL SIMULATED DRAWDOWNS WITH ANALYTICAL SOLUTION

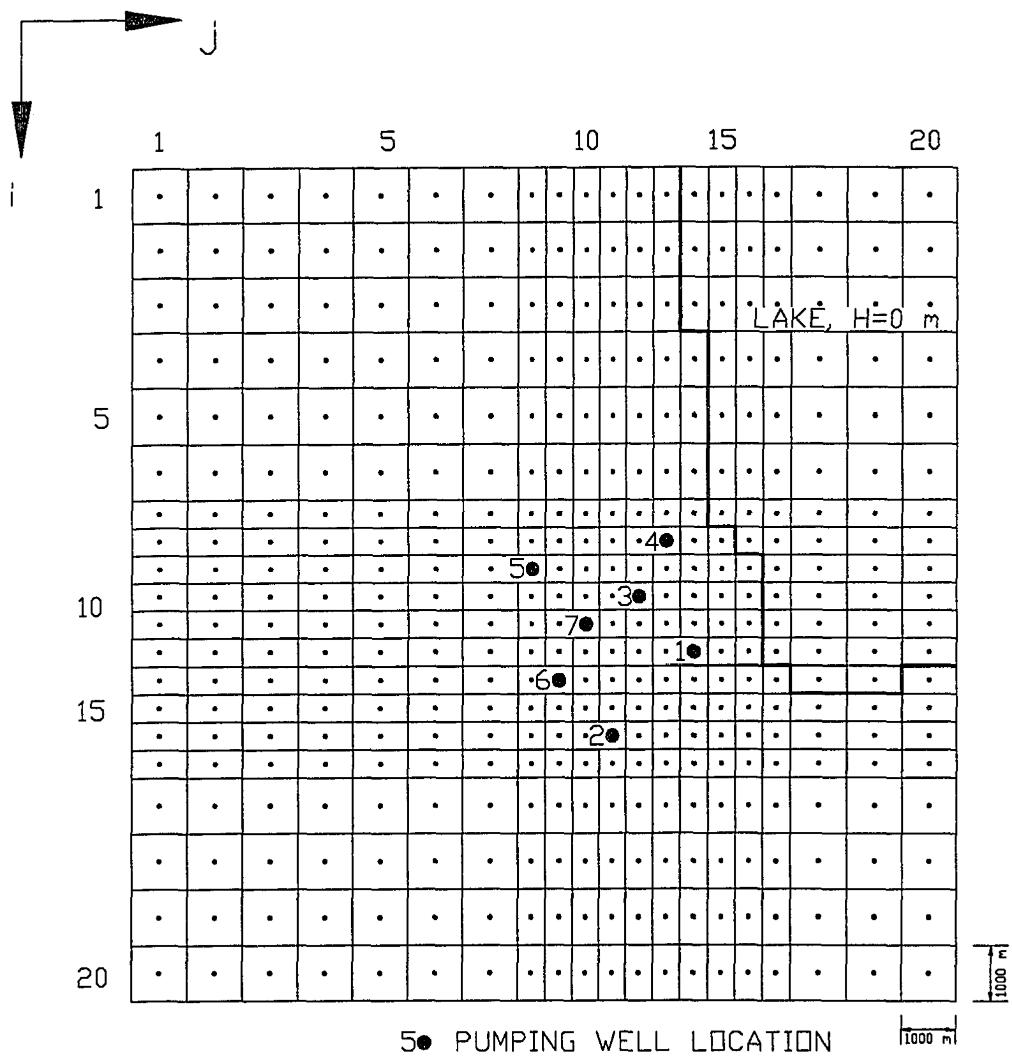


FIG. 4.3: FINITE DIFFERENCE GRID CONFIGURATION USED IN COMPARING NUMERICAL MODEL (FLOW COMPONENT) WITH PLASM

Boundary condition as defined in the Fig 4.3. Location of the wells are also shown in the figure. Discharge, Q from 7 Wells (in m^3/d) is given in Table 4.1.2.

Table 4.1.2

Pumping Well Discharges

YEAR	PW1	PW2	PW3	PW4	PW5	PW6	PW7
1	12100	14600	7000	7900	5000	5300	2300
2	13200	18200	9600	12100	5800	7300	3400
3	14300	21800	12200	16300	6600	9200	4000
4	15400	25400	14800	20500	7400	11200	4800
5	16500	29000	17400	24700	8200	13100	5700
6	17600	32600	20000	28900	9000	15100	6500
7	18700	36200	22600	33100	9800	17000	7400
8	19800	39800	25200	37300	10600	19000	8200
9	20900	43400	27800	41500	11400	21000	9000
10	22000	47000	30400	46700	12200	22400	10400

The model developed and PLASM were executed with the same set of data. The results obtained from the model (CCMODEL) and those obtained by executing PLASM are compared along a line parallel to X axis (Row 15) and along a line parallel to Y axis (Column 8). The aquifer heads obtained in time step 5 and time step 10 along Row 15 are graphically shown in Fig. 4.4 and those along Col 8 are shown in Fig. 4.5. As can be seen in Fig 4.4 and Fig 4.5 there is a very good agreement between the two numerical models. The piezometric head difference in the two models is within 1-2%, and this discrepancy is due to the convergence achieved in the two models.

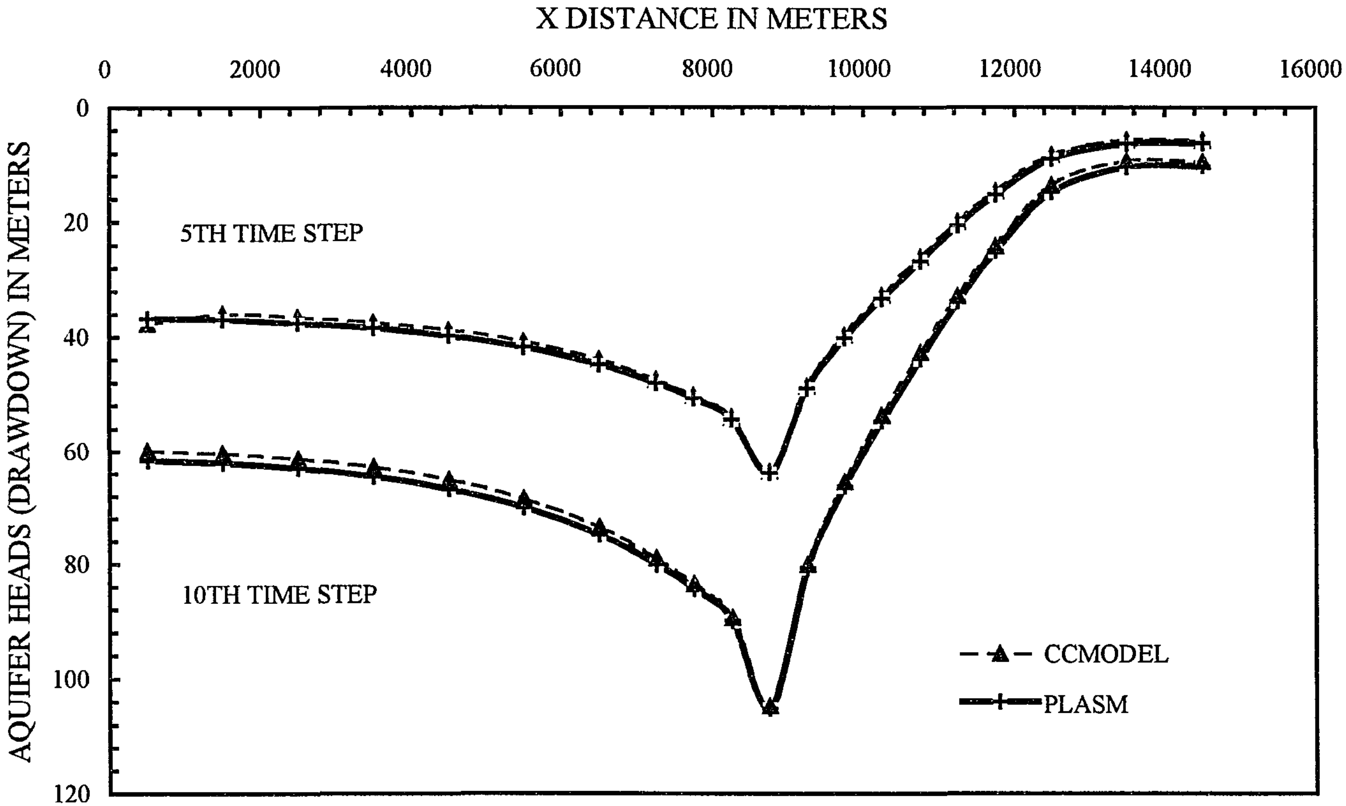


FIG 4.4: COMPARISON OF NUMERICAL MODEL SIMULATED DRAWDOWNS WITH NUMERICAL SOLUTION OBTAINED USING PLASM ALONG A LINE PARALLEL TO X AXIS

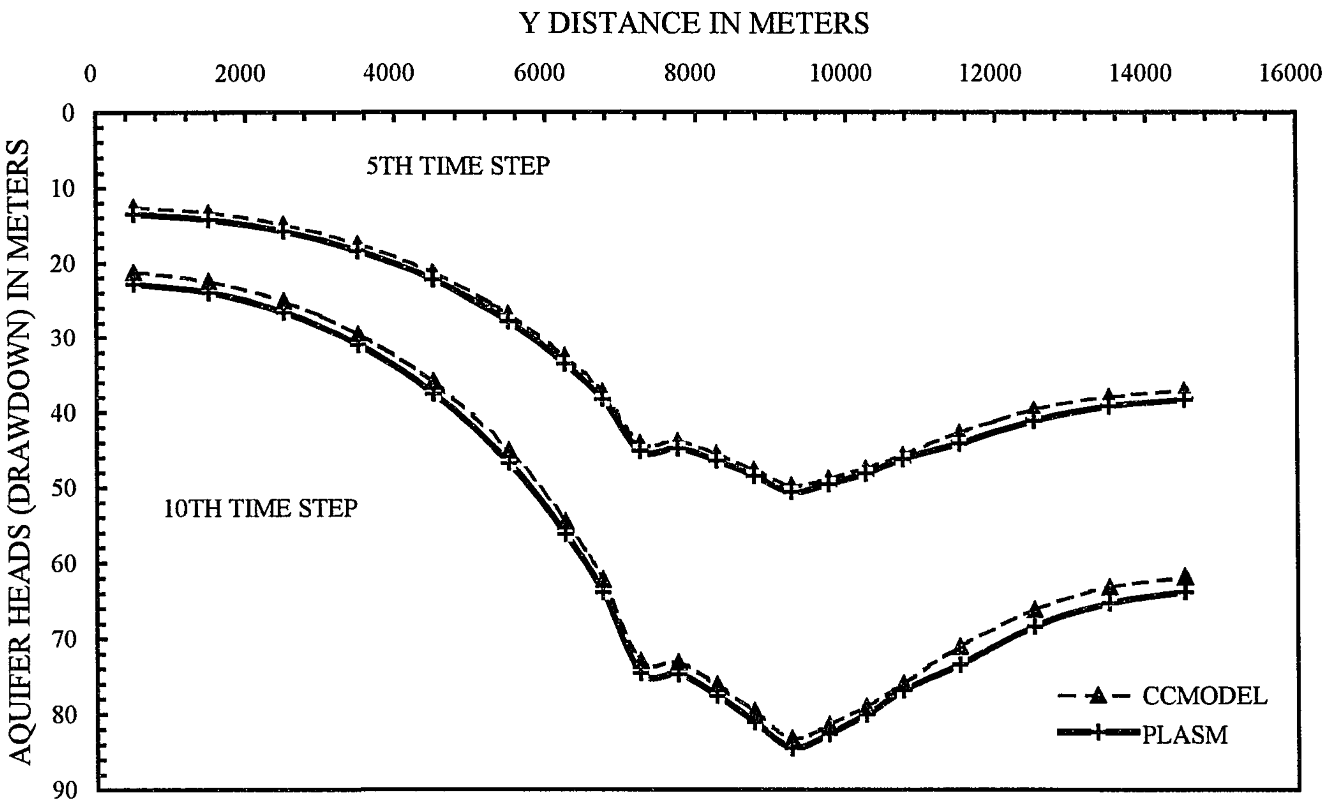


FIG 4.5: COMPARISON OF NUMERICAL MODEL SIMULATED DRAWDOWNS WITH NUMERICAL SOLUTION OBTAINED USING PLASM ALONG A LINE PARALLEL TO Y AXIS

4.1.5 Comparison of Model Generated Unit-Response Function with Analytical Solution

The analytical solution for the unit-response function for an unsteady, radial flow situation in an infinite, homogeneous, isotropic, non-leaky, confined aquifer, with a single well pumping Q_w^1 during the first time step t_1 and is then shut off permanently is given by (ref: Bear (1979), pp 323)

for $t \leq t_1$

$$s(r,t) = \frac{Q_w^1}{4\pi T} W(u), \qquad u = \frac{r^2 S}{4Tt} \tag{4.1.2}$$

for $t > t_1$

$$s(r,t) = \frac{Q_w^1}{4\pi T} \left[W(u) - W(u^*)\right], \qquad u^* = \frac{r^2 S}{4T(t-t_1)} \tag{4.1.3}$$

where r is the distance from the pumping well at any time t after the pumping has started, T = transmissivity, S = storage coefficient.

The input to the computer model to generate the unit-response function is tabulated below:

Aquifer Transmissivity, T	= 1000 m^2/d,
Storage Coefficient, S	= 0.001,
Grid Spacing $\Delta x = \Delta y$	= 300 m constant,
Density of Grid NROW = NCOL	= 49,
Time Step, Δt	= 30. d
Q (in first time period only)	= 1000 m^3/d
Pumping Well Location (i,j)	= (25,25)

Initial Piezometric Head, H_0 = 0.0 m throughout,

Barrier boundary condition on all four sides.

The comparison of analytical solution and unit-response function obtained by the model at the pumping well node (25,25) is shown in Fig. 4.6. The comparison of the model unit-response function shows very good agreement with theoretical solution.

4.1.6 Check for Principle of Superposition

The sample problem discussed in Section 4.1.5 is used to generate response function for three wells pumping at nodes (25,25), (20,20), and (34,28). Also, the response function was obtained at three observation nodes (25,26), (25,27), and (25,28). In the aquifer simulation constant discharges of 12000 m^3/d, 20000 m^3/d, and 8000 m^3/d was assigned for the three wells, respectively. The aquifer heads at the three pumping and three observation nodes are superposed as discussed in Section 3.4.3 (Eq. 3.4.2) and are compared with the simulated results in the computer program for every time step. Table 4.1.3 displays a comparison for the 13^{th} time step. In the Table 4.1.3, KP is point of interest, I and J refers to row and column numbers, respectively. The superposition achieved by using the unit-response function is quite satisfactory. The small discrepancy is principally due to convergence achieved in generating unit-response function for individual wells and in simulation the convergence achieved is for the combined pumping from all the wells.

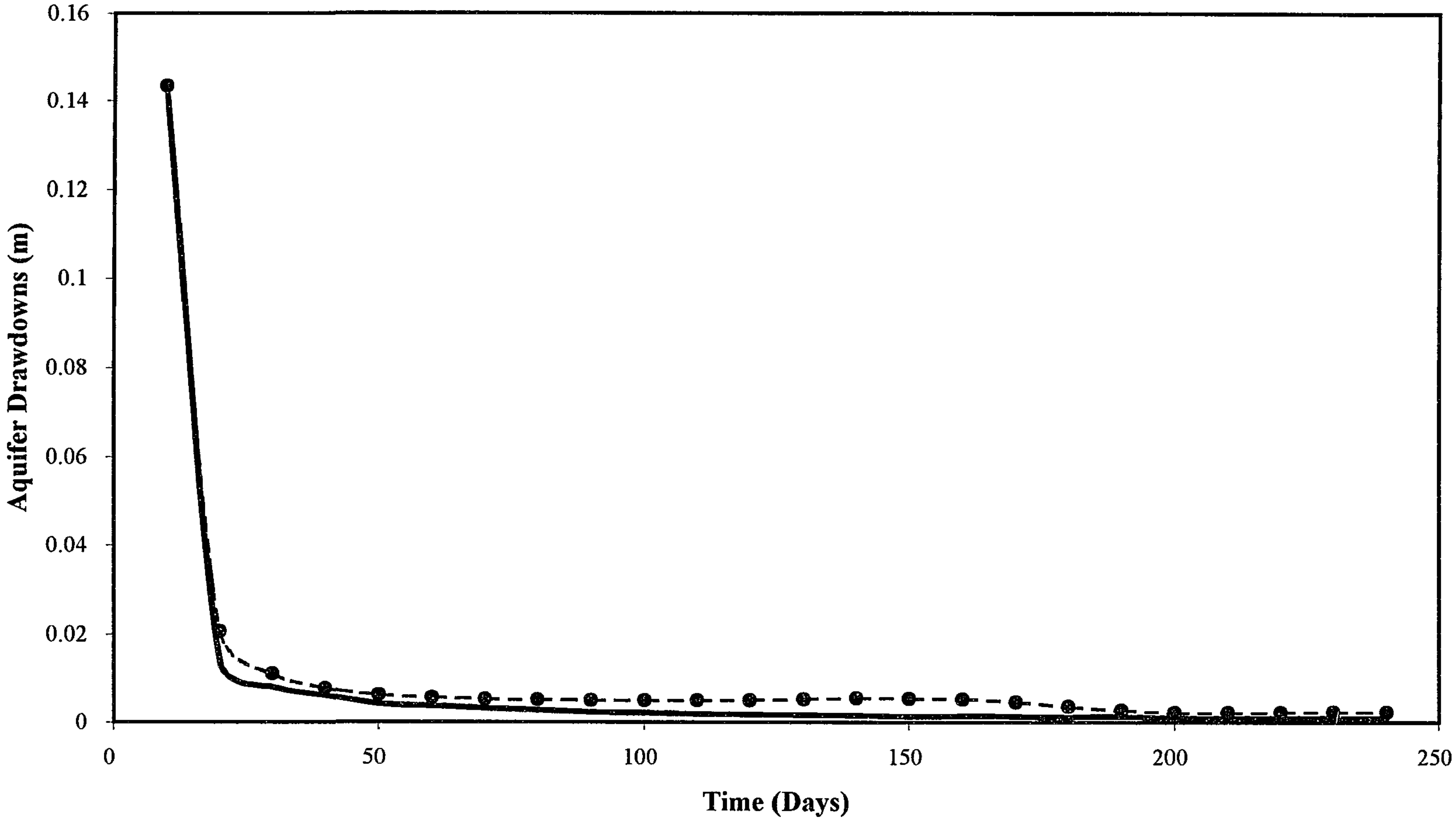


FIG 4.6: COMPARISON OF MODEL GENERATED URF WITH ANALYTICAL SOLUTION

Table 4.1.3

Comparison of Superimposed Heads and Simulated Heads

KP	I	J	Total s^* (m)	H (m) at KP	Head H^{**} (m)	Error	Remarks
1	25	25	3.0176	-3.0176	-3.0140	0.120%	Pump Well
2	20	20	4.0301	-4.0301	-4.0261	0.100%	Pump Well
3	34	28	1.9468	-1.9468	-1.9459	0.044%	Pump Well
4	25	26	2.2070	-2.2070	-2.2036	0.155%	Obs. Well
5	25	27	1.8091	-1.8091	-1.8059	0.175%	Obs. Well
6	25	28	1.5538	-1.5538	-1.5510	0.185%	Obs. Well

Note : * Indicates the total drawdown (m) computed using the Eq. 3.4.2

: ** Indicates the simulated head using the aquifer simulation program developed.

4.2 VERIFICATION OF STOCHASTIC GENERATION OF AQUIFER PARAMETERS

Several intermediate steps were printed in the course of model development which were all checked by hand calculations for small size problems. In the stochastic component of the model developed many useful routines for matrix decomposition, back substitution, eigen value and eigen vector generation, reduction of symmetric matrix into tridiagonal form, and generation of random numbers which are normally distributed with mean 0 and variance 1 are all standard FORTRAN subroutines from the book titled "Numerical Recipes: The Art of Scientific Computing" by Press et al. (1992).

4.2.1 Check for Optimum Values of MLE Parameters

An internal check is accomplished by back substituting the optimum MLE parameters in the likelihood equation. It is found that the optimum MLE parameters have consistently satisfied the likelihood equation (Eq. 3.3.7), i.e. the derivative of the negative log likelihood function with respect to each structural parameter, θ_j, is equal to zero.

$$\frac{\partial L}{\partial \theta_j} = 0$$

where θ_j can be any of the structural parameters, mean μ, variance σ^2, correlation length scale λ_x or λ_y.

This internal running check is printed for each hydrogeologic parameter after optimum values of the vector of unknown spatial statistical structural parameters of the log parameter field is determined using the MLE procedure discussed in Section 3.3.1. The sample of the same is reproduced in Table 4.2.1. The results shown in Table 4.2.1 correspond to the data used in estimating random log field for permeability in the Y direction of Region 2 discussed in Section 5.1.1.2. As seen in Table 4.2.1, the value of the gradient vector is very close to zero that means the likelihood equations given in Eq. 3.3.7 and mentioned above are satisfied. The small discrepancy in the gradient vector is acceptable because of the convergence criterion specified in the MLE procedure. Mean and variance given in Table 4.2.1 are the logarithmic values of the random field.

Table 4.2.1

Optimum MLE Parameters

Structural Parameter	Optimum Value	Gradient Vector	Value
μ	1.52103	$\frac{\partial L}{\partial \mu}$	0.017
σ^2	0.04174	$\frac{\partial L}{\partial \sigma^2}$	0.012
λ_x	2389.1	$\frac{\partial L}{\partial \lambda_x}$	0.000
λ_y	2487.9	$\frac{\partial L}{\partial \lambda_y}$	0.000

The non-linear optimization method developed here for estimating the optimum MLE parameters, is an iterative process. During each iteration the corrections for all the four structural parameters are employed simultaneously using matrix methods as discussed in Appendix A1. The optimum MLE parameters obtained was in agreement with optimum MLE parameters obtained using another approach known as "Profile Method" which was developed in the initial stages of this study. Essentially, the profile method is also an iterative process. In the profile method the corrections for each structural parameters are employed individually, and the updated or corrected parameters are used in employing correction for the other structural parameters, and the iterations are continued until convergence criteria is met. The non-linear optimization method was later developed because of its inherent computational efficiency.

4.3 VERIFICATION OF SURFACE WATER FLOW COMPONENT

The non-linear hydrologic storage equation described in Eq. 3.5.12 is embedded in the non-linear optimization model developed as discussed previously. In the optimization procedure these are strict equality constraints. The optimum solution is obtained only after satisfying the equality constraints.

4.3.1 Check for Mass Balance

As a check for mass balance for each reach in each time step is printed in the output, and the same for a sample problem is reproduced here in Table 4.3.1. The data input to the sample problem is same used in model application discussed in Section 5.1.2.1. In Table 4.3.1 ΣQ_{in} is the sum of upstream (U/S) inflow plus any waste flow input to the reach and ΣQ_{out} is the sum of downstream (D/S) outflow plus diversion from the reach plus induced infiltration. Only for presentation purpose here the percent error is calculated as (ΣQ_{in} - ΣQ_{out}) divided by ΣQ_{in} times 100. In the model the stream mass balance equations (Eq. 3.5.12) are modeled as strict non-linear equality constraints. The optimum solution obtained satisfies these equality constraints.

Table 4.3.1

Check for Streamflow Mass Balance

Reach #	Stream Depth (m)	U/S Qin (1000 m^3/d)	D/S Qout (1000 m^3/d)	Diversion (1000 m^3/d)	Infiltration (m^3/d)	Waste flow Input(1000 m^3/d)	$\sum$ Qin - $\sum$ Qout (m^3/d)	Error %
1	21.0915	35622.0	35621.7	0.0	-275.	0.0	12.	0.00
2	21.0915	35621.7	35621.6	0.0	-139.	0.0	8.	0.00
3	21.0914	35621.6	35621.4	0.0	-199.	0.0	4.	0.00
4	21.0914	35621.4	35621.2	0.0	-160.	0.0	16.	0.00
5	21.0913	35621.2	35621.1	0.0	-119.	0.0	8.	0.00
6	21.0913	35621.1	35620.9	0.0	-87.	0.0	24.	0.00
7	21.0206	35620.9	35421.9	198.8	-41.	0.0	170.06	0.00
8	21.0206	35421.9	35421.9	0.0	+24.	0.0	40.00	0.00
9	21.0206	35421.9	35421.9	0.0	+12.	0.0	20.00	0.00
10	21.0206	35421.9	35421.9	0.0	+4.	0.0	24.00	0.00
11	21.0206	35421.8	35421.9	0.0	+4.	0.0	20.00	0.00
12	21.0384	35421.8	35471.8	0.0	+1.	50.0	20.00	0.00
13	21.0384	35471.8	35471.8	0.0	+4.	0.0	8.00	0.00
14	21.0384	35471.8	35471.8	0.0	+23.	0.0	20.00	0.00
15	21.0384	35471.8	35471.9	0.0	+23.	0.0	8.00	0.00
16	21.0384	35471.9	35471.9	0.0	+37.	0.0	16.00	0.00
17	21.0384	35471.9	35472.0	0.0	+143.	0.0	12.00	0.00

4.4 VERIFICATION OF THE GROUNDWATER SOLUTE TRANSPORT COMPONENT

In verifying the groundwater solute transport component several tests were conducted. These tests are discussed individually below:

4.4.1 Check for Mass Balance

This is an internal running check for all time steps. Mass balance in solute transport component is defined as mass present in the system should equal the difference of all mass input/inflow and mass pumped/outflow of the system. The check for mass balance is printed in the computer output for every time step, and the sample of the same (for the problem discussed in Section 4.4.6, Time Step 16) is shown in Table 4.4.1.

Table 4.4.1

Check for Mass Balance - Solute Transport Component

Mass Injected from Start	630.0 Tons
Mass Recharged from Boundary	-11.19 Tons
Total Mass In	618.81 Tons
Mass Present in the System	605.43 Tons
Mass Removed from Pumping Wells	13.38 Tons
Total Mass Out	618.81 Tons
MASS BALANCE ERROR	0.00001%

4.4.2 Check for Symmetric Distribution of Concentration

A hypothetical homogeneous, and isotropic aquifer is considered with symmetric boundary conditions. Four pumping wells and one injection well are placed symmetrically in the aquifer. The size of the aquifer, boundary and initial conditions, governing parameters for flow is the same as given in Section 4.1.2. The aquifer is discretized into 31 rows x 31 columns of equal grid spacing of 300 m. Constant discharge of 10000 m^3/d at the four pumping wells located at nodes (16,13), (16,19), (13,16), and (19,16) is used. The injection well is located at the center of the aquifer at node (16,16) with a constant injection rate of 20000 m^3/d. The porosity of the porous medium = 0.1, and a constant dispersivity of 10 m is assumed in both X and Y direction. The distribution of concentration in the aquifer is found to be symmetric using all the methods (centered, upwind, weighted, and quadratic interpolation finite difference methods) developed in this study. In the upwind weighted difference method, weight w = 0.75 is used here and in all other comparisons. The symmetric distribution of concentrations obtained using quadratic interpolation method along a line parallel to X axis is shown in Fig. 4.7, and along a line parallel to Y axis is shown in Fig. 4.8.

4.4.3 Comparison of Model Results with Analytical Solution for Axially Symmetric Steady Flow Field

The analytical solution for concentrations in an infinite aquifer for radially symmetric diverging flow from a well continuously injecting a tracer at constant rate Q_0 and constant concentration C_o is given by (ref: Bear 1972, pp 635)

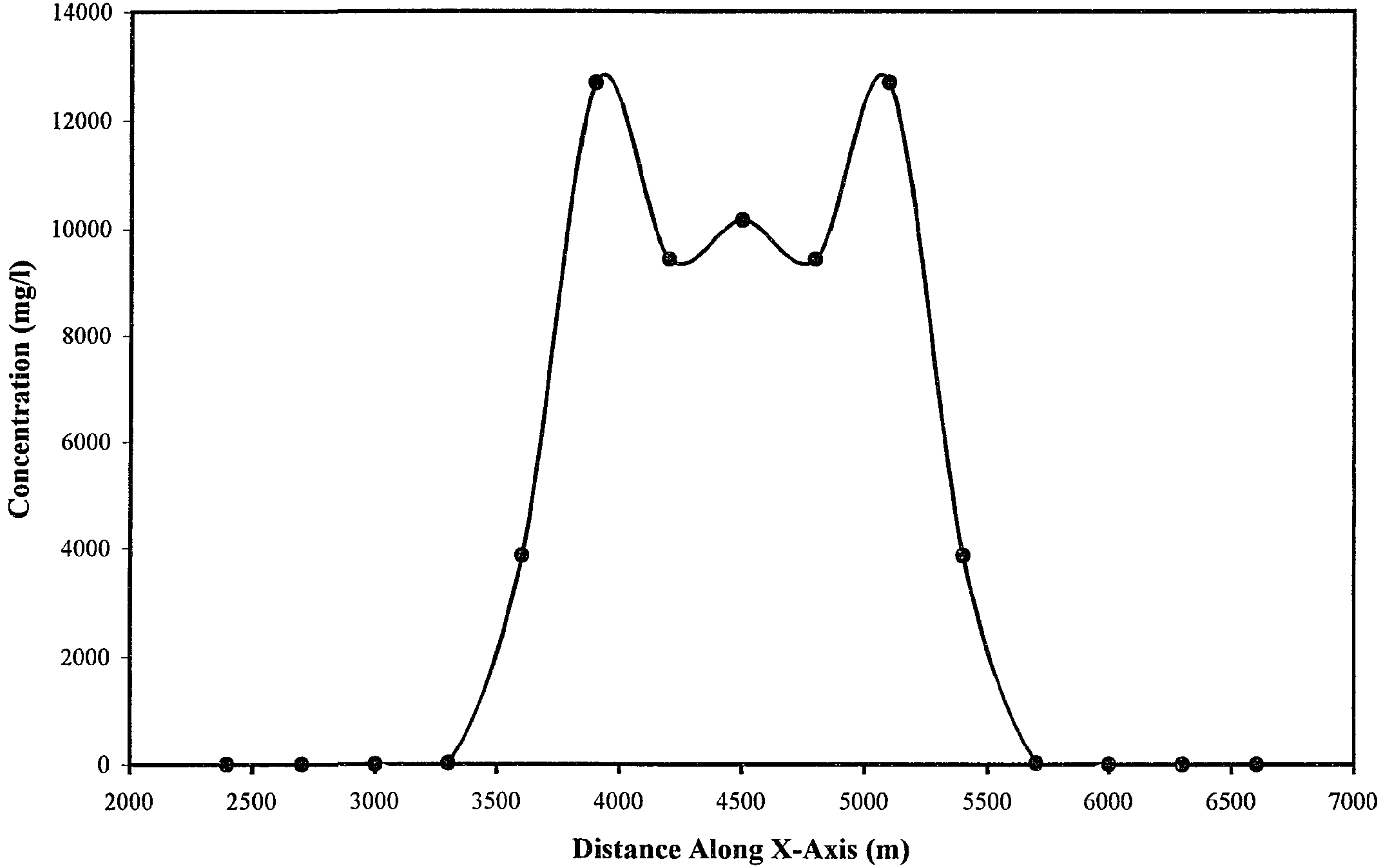


FIG 4.7: CHECKING FOR AXIAL SYMMETRY ALONG A LINE PARALLEL TO X AXIS

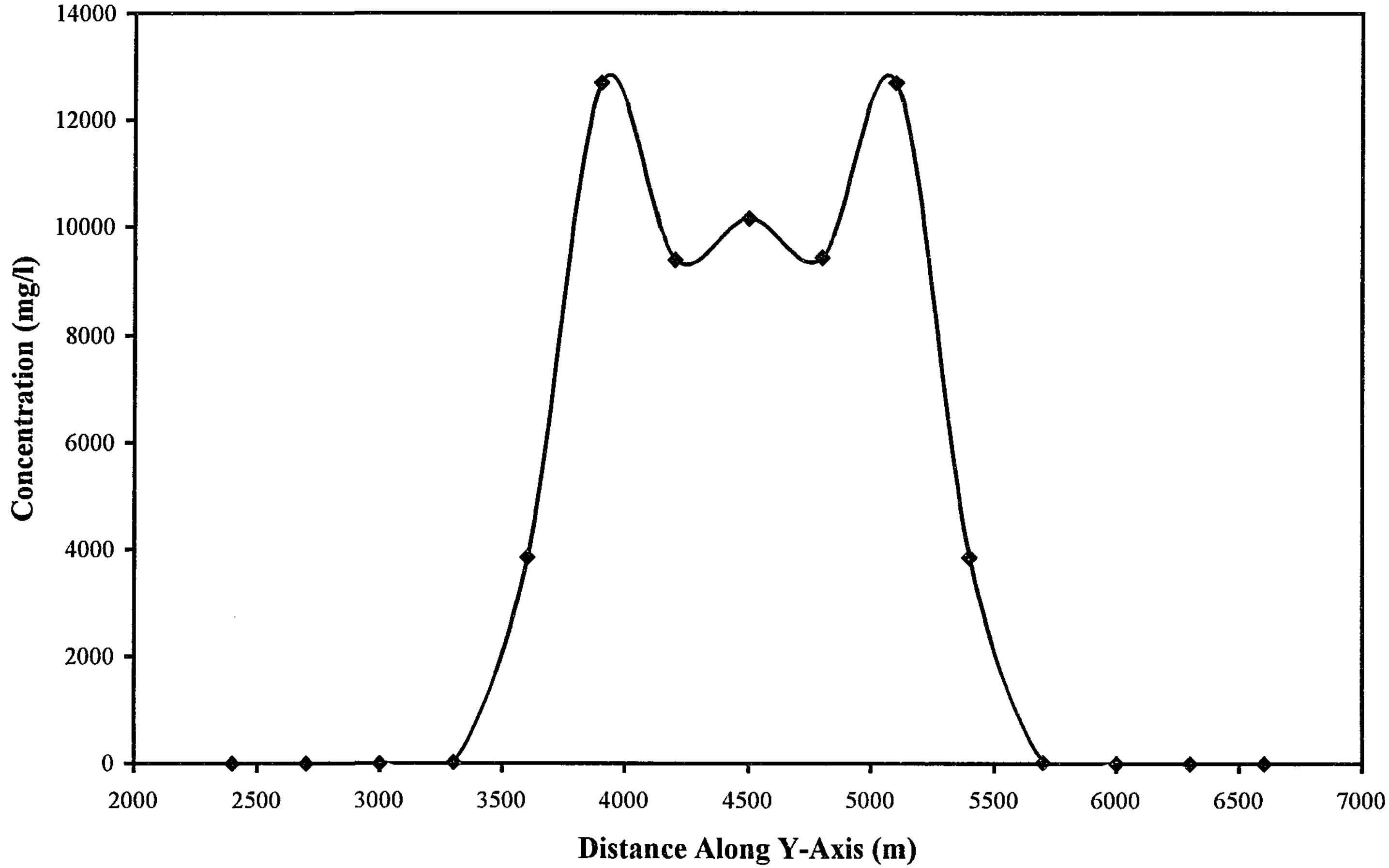


FIG 4.8: CHECKING FOR AXIAL SYMMETRY ALONG A LINE PARALLEL TO Y AXIS

$$C(r,t) = \frac{C_o}{2}\, erfc\left(\frac{\frac{r^2}{2} - Gt}{\sqrt{\frac{4}{3}\,\alpha_L \bar{r}^3}}\right) \tag{4.4.1}$$

where

$$G = \frac{Q_o}{2\pi B\phi} = V\,r \tag{4.4.2}$$

$\bar{r}$ is the average radius of the body of injected mass and defined as $\bar{r} = \sqrt{2Gt}$, and r is the radial distance from the center of the well.

This analytical solution is used to test the mathematical model developed. The input to the model consisted of constant injection rate Q_o = 1 m^3/s and constant concentration C_o = 1000 g/m^3, $\Delta x = \Delta y =$ 40 m constant, NROW = NCOL = 101, Source location (i,j) = (51,51) and barrier boundary condition on all sides, time step Δt = 34646.4 s, thickness of the aquifer = 10 m, constant permeability in X and Y direction of 0.0005 m/s, porosity = 0.35, and a constant dispersivity in X and Y direction of 10 m.

Numerical results obtained using all the schemes (centered, upwind, weighted, and quadratic interpolation finite difference methods) are compared with analytical solution. The comparison of relative concentration (C/C_o) versus radial distance after 4.01 days and after 36.10 days using quadratic interpolation method is shown in Fig. 4.9. In the Fig. 4.9, QUI stand for quadratic upstream interpolation scheme. The numerical results obtained using centered, upwind, and weighted difference methods are compared in Fig. 4.10. In the Fig. 4.10, CDM, UDM, and WDM stand for centered, upwind, and weighted upwind difference schemes, respectively. Same notations are used in all other comparisons.

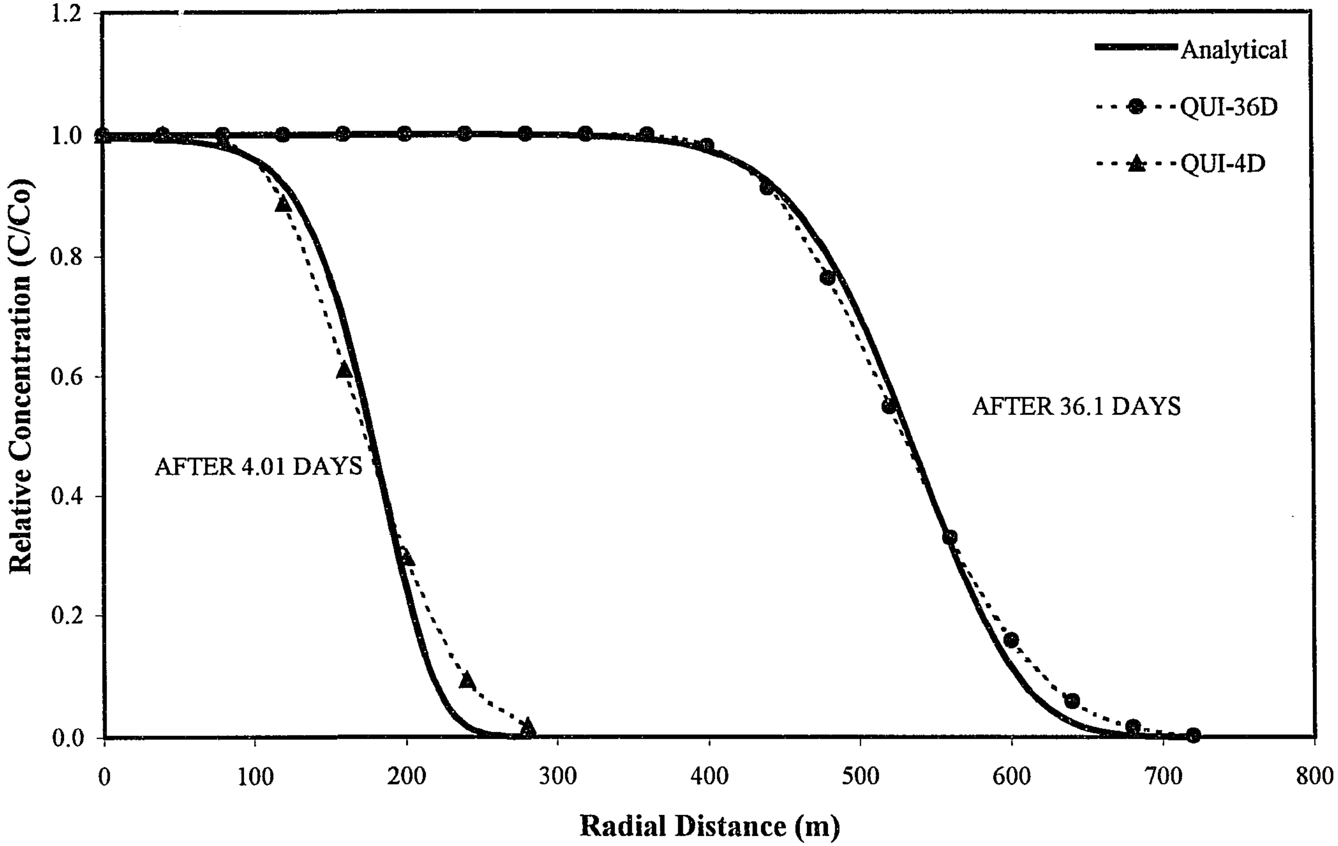


FIG 4.9: COMPARISON OF NUMERICAL RESULTS OBTAINED USING QUADRATIC UPSTREAM INTERPOLATION METHOD WITH ANALYTICAL SOLUTION FOR 2D DIVERGING FLOW

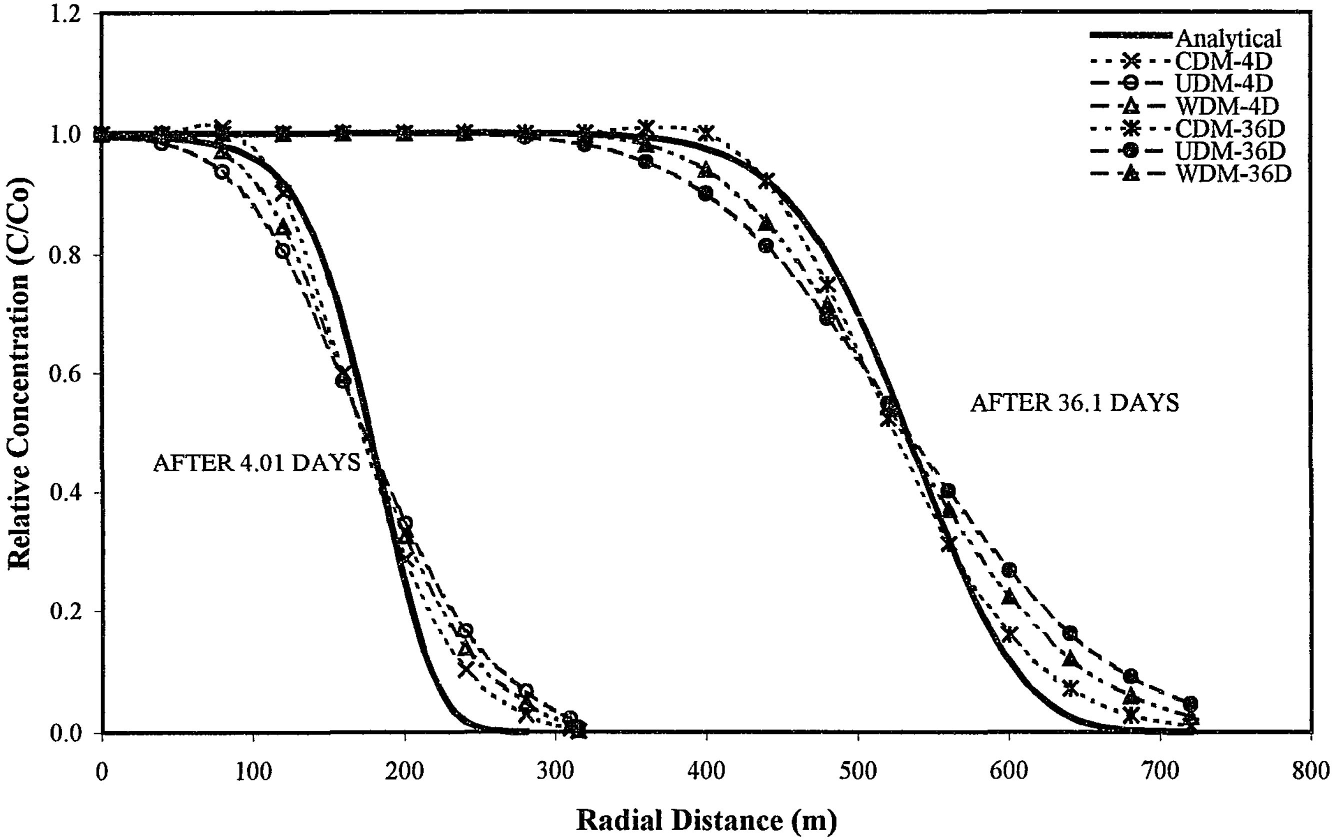


FIG 4.10: COMPARISON OF NUMERICAL RESULTS OBTAINED USING CENTRAL, UPWIND, AND WEIGHTED DIFFERENCE METHOD WITH ANALYTICAL SOLUTION FOR 2D DIVERGING FLOW

The application of the model which is written essentially for two-dimensional Cartesian coordinates, to a problem involving radially symmetric divergent flow field represents a severe test of the model. Nevertheless, it can be seen in Fig. 4.9 that there is good agreement between analytical and numerical solutions after both relatively short and long times. Further, it can be seen in both cases (after 4.01 days and after 36.1 days) that quadratic interpolation method closely follows analytical solution. However, the presence of some numerical dispersion is evident (ref to Fig. 4.10), particularly for the longer time when upwind or weighted difference methods are used.

4.4.4 Comparison of Model Results With Analytical Solution for Steady Uniform Flow Field

The analytical solution for a homogeneous, isotropic, infinite aquifer with a uniform flow in one direction parallel to the axis and of constant velocity, U, for the case of instantaneous injection (momentary injection) of concentration ΔM at the origin (x=0, y=0) at time t = 0, is given by Kinzelbach, 1986

$$C(x,y,t) = \frac{\Delta M}{4\pi\phi B U\sqrt{\alpha_L \alpha_T}\, t} \exp\left(- \frac{\left(x - \frac{Ut}{R}\right)^2}{4\alpha_L \frac{Ut}{R}} - \frac{y^2}{4\alpha_T \frac{Ut}{R}} \right) \exp(-\lambda t) \tag{4.4.3}$$

where λ is the decay constant, α_L and α_T are longitudinal and transverse dispersivities, R is the retardation factor.

To test the model with this analytical solution a 290 m x 290 m aquifer is considered. The aquifer is discretized by a constant grid spacing of $\Delta x = \Delta y = 10$ m. A momentary injection of 200 kg of an ideal tracer (R = 1, $\lambda = 0$) is applied at

location (50 m, 150 m). A time step of $\Delta t = 1.0$ day is used. The aquifer is assumed to be homogeneous with $K_x = K_y = 28$ m/d; constant thickness B = 10 m; aquifer porosity $\phi = 0.1$, dispersivities $\alpha_L = 4.5$ m and $\alpha_T = 1.125$ m. The uniform flow field with pore velocity of U = 1.0 m/d is defined by setting a constant head boundary on left and right edges of the aquifer with $h_L = 100.0$ m and $h_R = 99.0$ m, respectively, and barrier boundary on other two edges. The dimension parameter statement in the computer program was modified to account for 125 time steps.

The comparison of the numerical results obtained using quadratic upstream interpolation with analytical solution after 120 days is shown in Fig. 4.11, and the same comparison using centered, upwind, and weighted difference methods is shown in Fig. 4.12. As can be seen in the Fig. 4.11, and Fig. 4.12 there is a very good agreement of the results obtained using quadratic interpolation and centered finite difference methods with analytical solution. However, a significant numerical dispersion is evident (see Fig. 4.12) when upwind or weighted difference methods are used. In Fig. 4.11, and Fig. 4.12 the concentration of the injected mass has moved with the velocity (U/R = 1.0 m/d) and the peak concentration in all the methods is obtained at a distance (Ut/R = 120 m) from the source location. Further, it should be noted that the constant velocities ($U_x = 1.0$ m/d and $U_y = 0.0$ m/d) as defined in the analytical solution can not be obtained everywhere in the mathematical model because of the radial velocities caused by the source injection. However, the discrepancy between velocities used in the analytical and mathematical model were negligible. Additionally, model boundaries though placed far from the source may still have some influence on the results. However, a much larger grid with NROW = NCOL = 49 was tested to eliminate this effect, if any, but the accuracy of the results

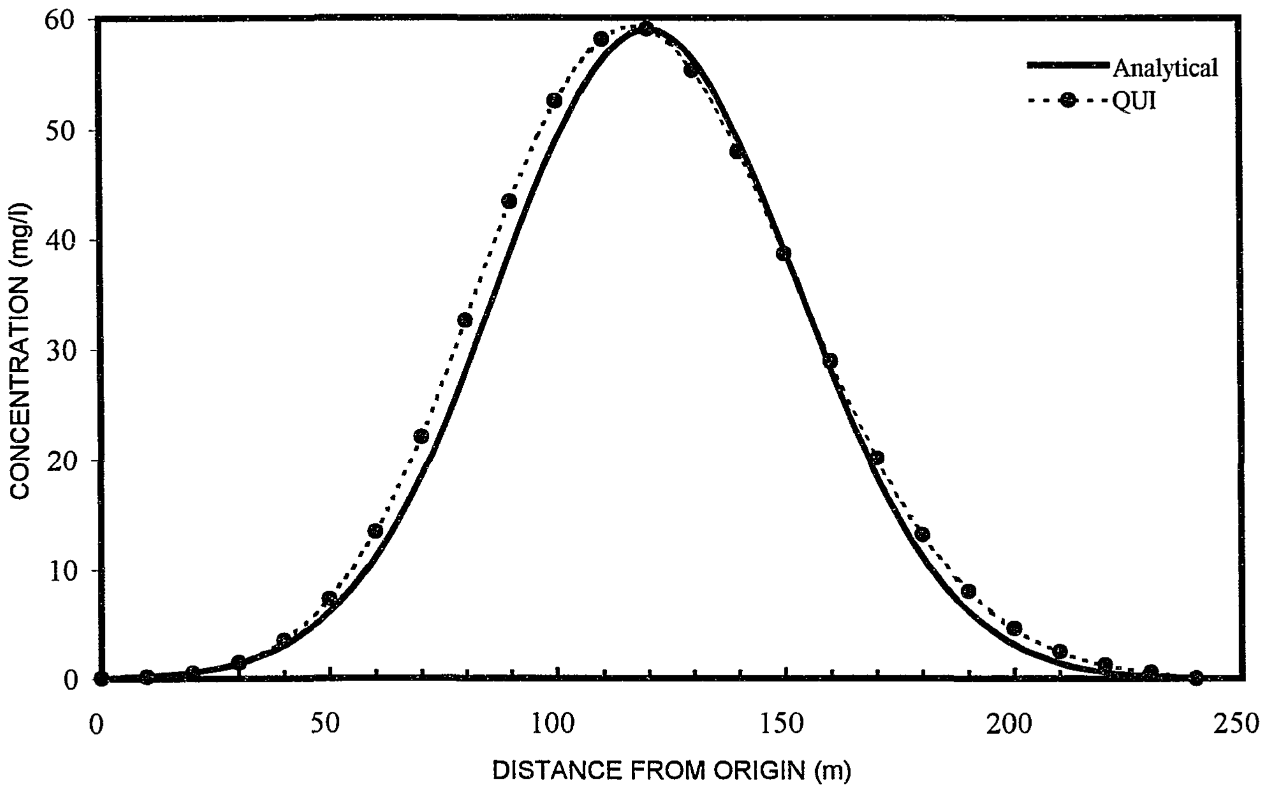


FIG 4.11: COMPARISON OF NUMERICAL RESULTS OBTAINED USING QUADRATIC UPSTREAM INTERPOLATION WITH ANALYTICAL SOLUTION - STEADY UNIFORM FLOW

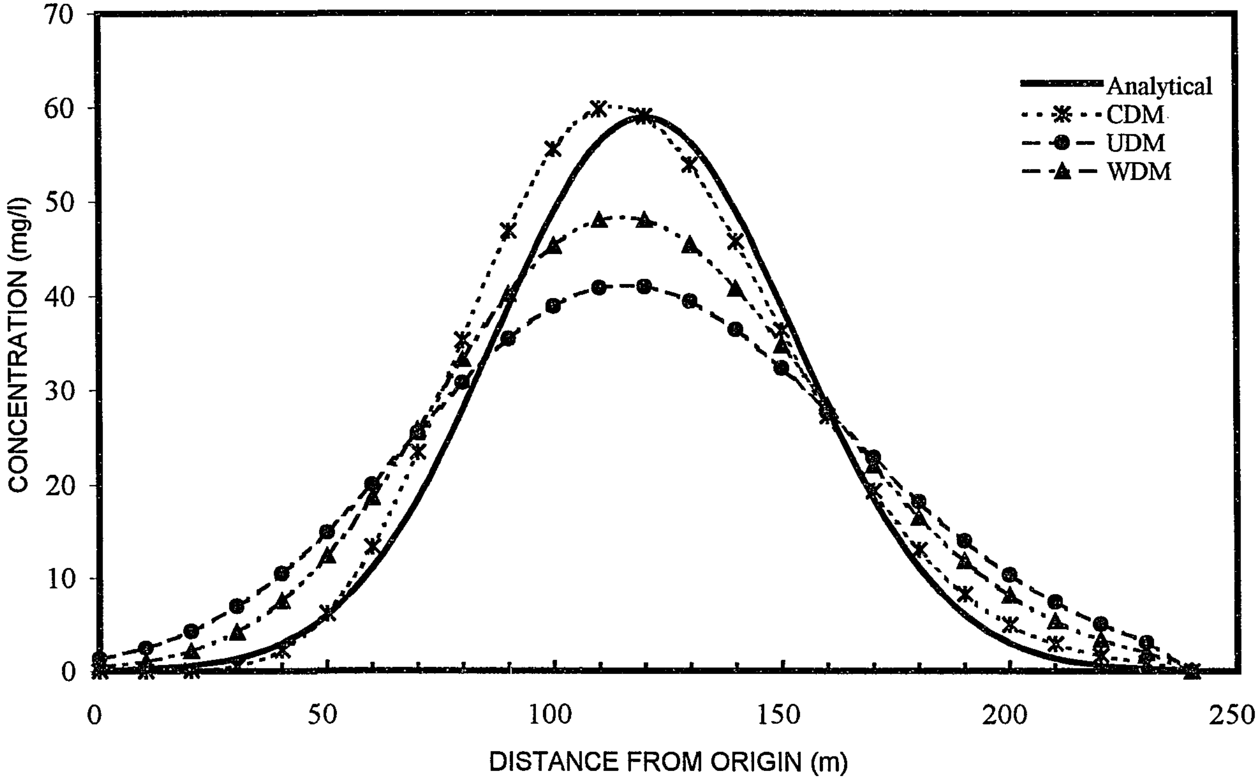


FIG 4.12: COMPARISON OF NUMERICAL RESULTS OBTAINED USING CENTRAL, UPWIND, AND WEIGHTED DIFFERENCE METHOD WITH ANALYTICAL SOLUTION - STEADY UNIFORM FLOW

were not affected. Therefore it can be said in the demonstrated model there was no boundary effects to distort the results.

4.4.5 Comparison of Model Results With Method of Characteristics (MOC) Solution

Konikow and Bredehoeft (1978) evaluated their solute transport model developed using Method of Characteristics (MOC) technique by applying it to a problem in which the flow field is strongly influenced by pumping wells. Fig. 4.13 shows the finite difference grid configuration of the aquifer model used in this application.

The input to the computer model is tabulated below:

Aquifer Transmissivity, T		= 802.66 m^2/d,
Storage Coefficient, S		= 0.00,
Grid Spacing $\Delta x = \Delta y$		= 274.3 m constant,
Density of Grid	NROW	= 8,
	NCOL	= 7,
Time Step, Δt		= 48.06 d
Constant well discharge, Q		= 2446.58 m^3/d
Pumping Well Location (i,j) = (6,3)		
Constant head boundary,	h_T	= 30.48 m
	h_B	= 22.86 m
Barrier boundary condition on other two sides		
Aquifer porosity, ϕ		= 0.30
Longitudinal Dispersivity,	α_L	= 30.48 m

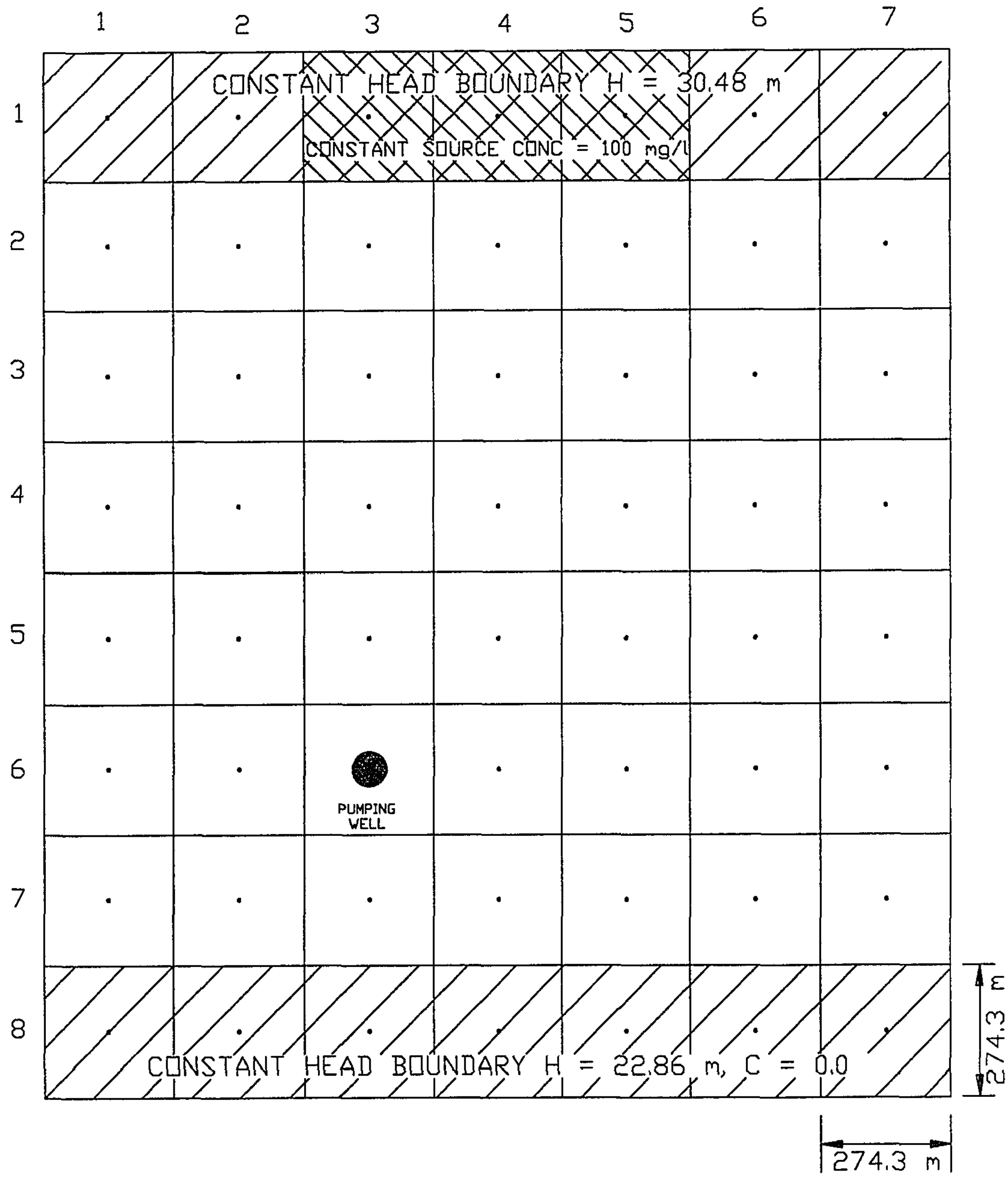


FIG. 4.13: FINITE DIFFERENCE GRID CONFIGURATION USED IN COMPARING NUMERICAL MODEL (SOLUTE TRANSPORT COMPONENT) WITH MOC

Transverse Dispersivity, α_T = 9.144 m

Constant Concentration of 100 mg/l at top central 3 nodes

The mathematical model developed in this study is applied to the same situation and the results are compared to those of Konikow and Bredehoeft (1978). The comparison of concentration distribution obtained using quadratic interpolation method along a line parallel to X-axis (Row 6) and along a line parallel to Y-axis (Column 3) is graphically presented in Fig. 4.14 and Fig. 4.15, respectively. A similar comparison is made of the numerical results obtained using centered, upwind, and weighted difference methods and these are shown in Fig. 4.16, and Fig. 4.17. Although the agreement of numerical results is very good, it should be noted that close to model boundaries there is some significant difference. This may be attributed to the different ways, in which the boundaries are represented in the two models. As can be seen in Fig. 4.15 (along Column 3) the MOC numerical results do not strictly maintain the constant boundary conditions specified. However, the concentration at the pumping well is in strict agreement with MOC solution irrespective of the difference method used i.e. quadratic, centered, upwind, and weighted difference methods. As mentioned in Section 3.6.3.4, for preliminary engineering analysis the centered, upwind, and weighted difference methods developed in this research work to model advective component are useful and produces global correspondence with measured results. However, the quadratic upstream interpolation scheme is the most accurate.

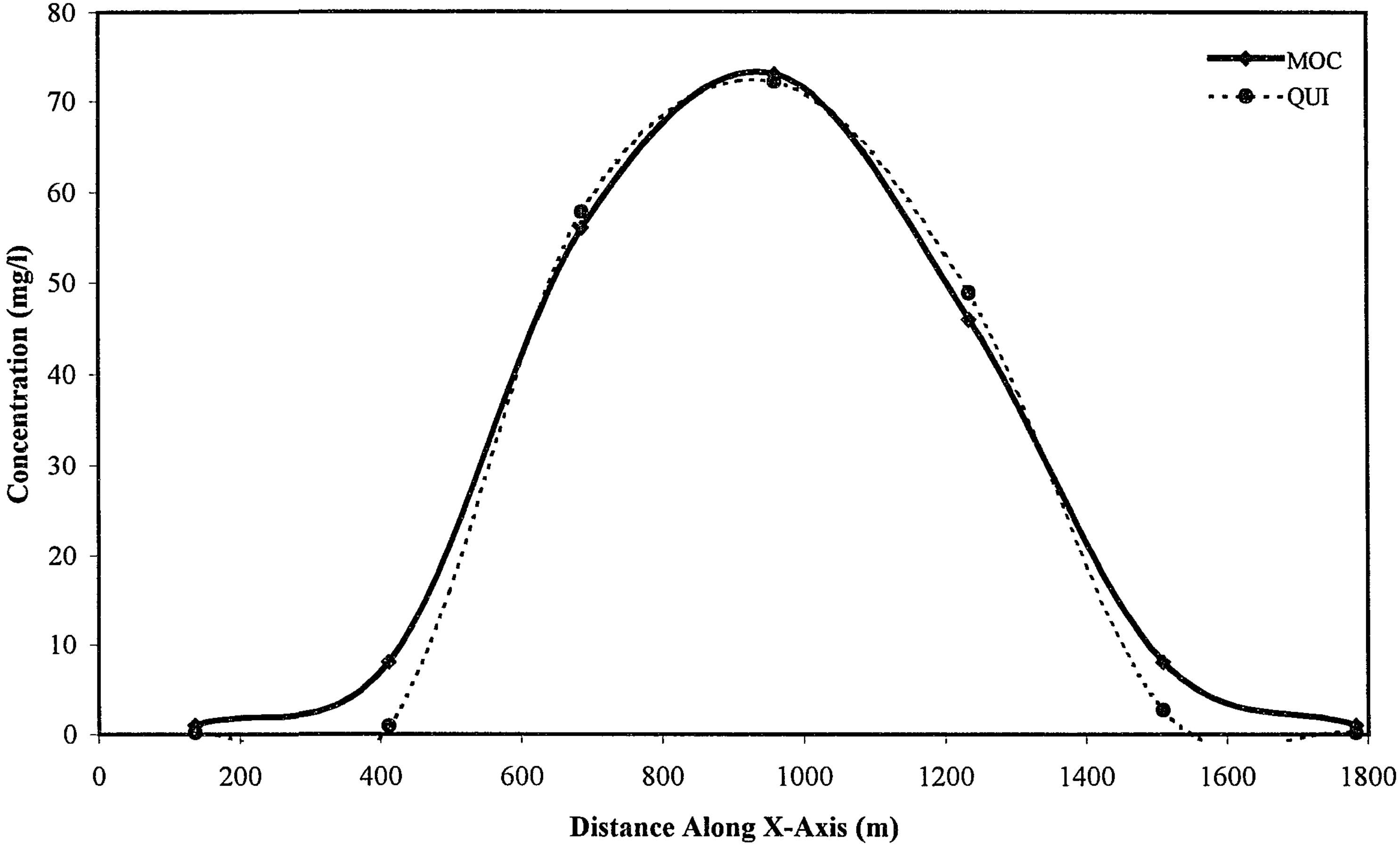


FIG 4.14: COMPARISON OF CONCENTRATION DISTRIBUTION OBTAINED USING QUADRATIC UPSTREAM INTERPOLATION WITH MOC SOLUTION ALONG A LINE PARALLEL TO X AXIS

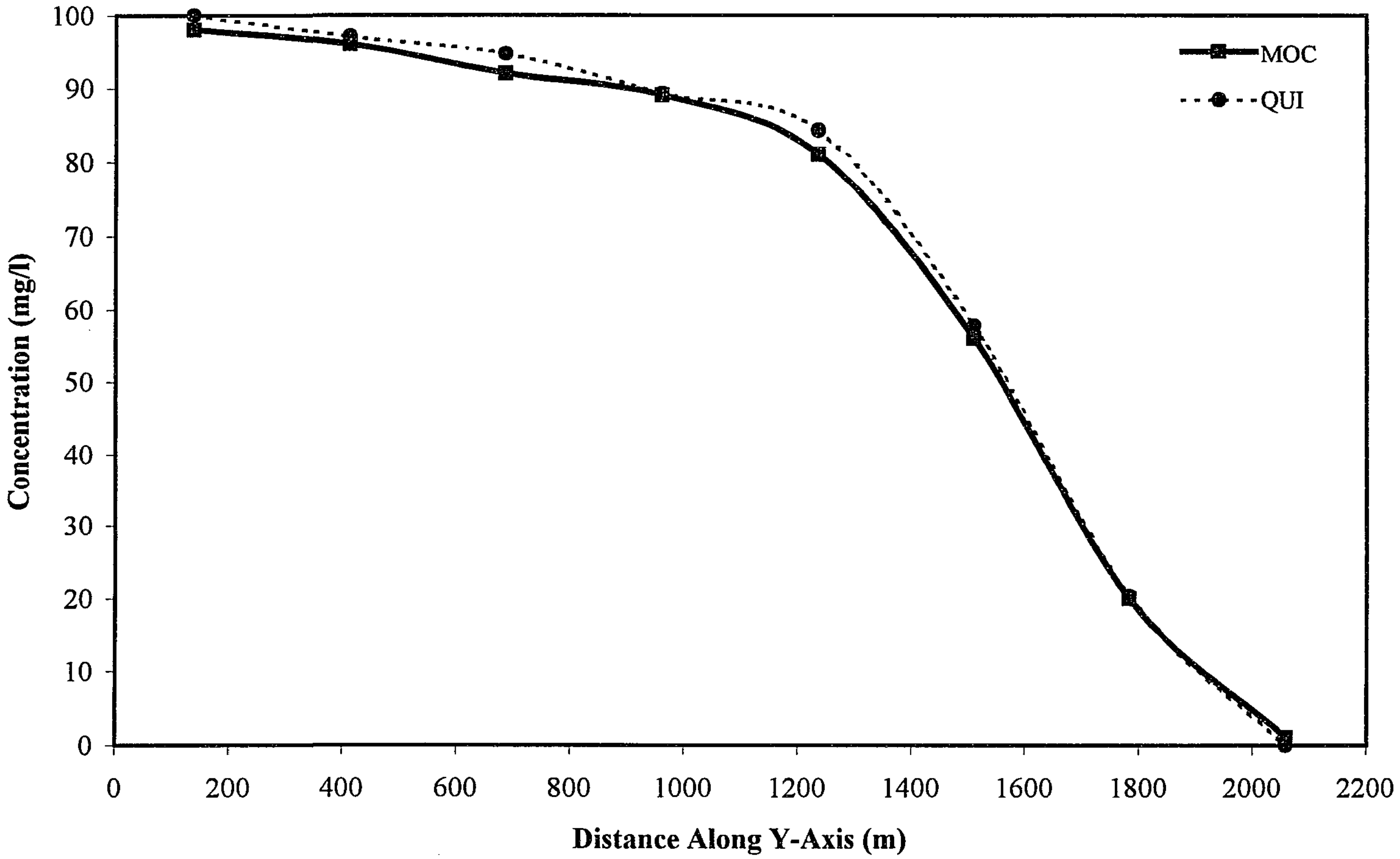


FIG 4.15: COMPARISON OF CONCENTRATION DISTRIBUTION OBTAINED USING QUADRATIC UPSTREAM INTERPOLATION WITH MOC SOLUTION ALONG A LINE PARALLEL TO Y AXIS

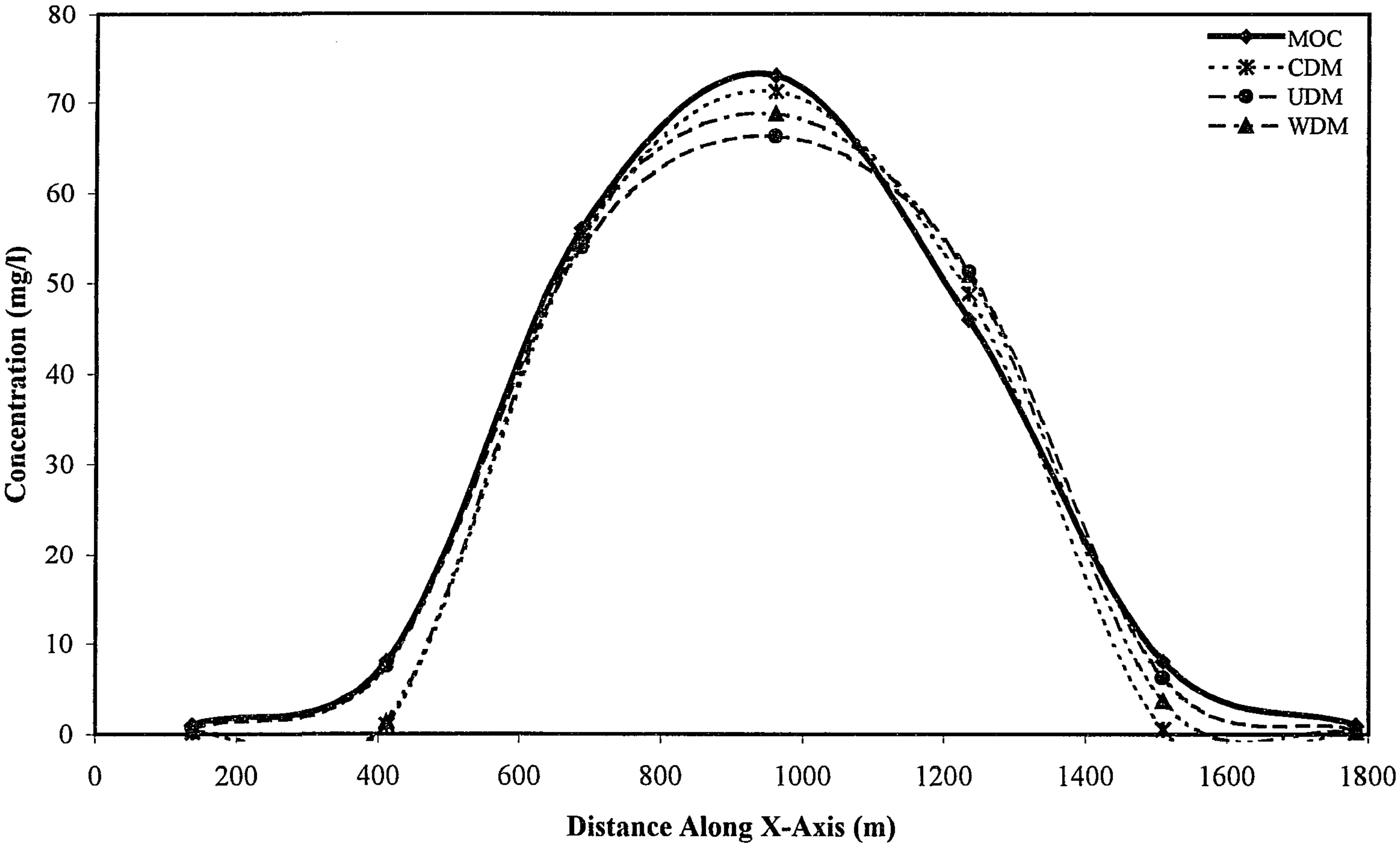


FIG 4.16: COMPARISON OF CONCENTRATION DISTRIBUTION OBTAINED USING CENTRAL, UPWIND, AND WEIGHTED DIFFERENCE WITH MOC SOLUTION ALONG A LINE PARALLEL TO X AXIS

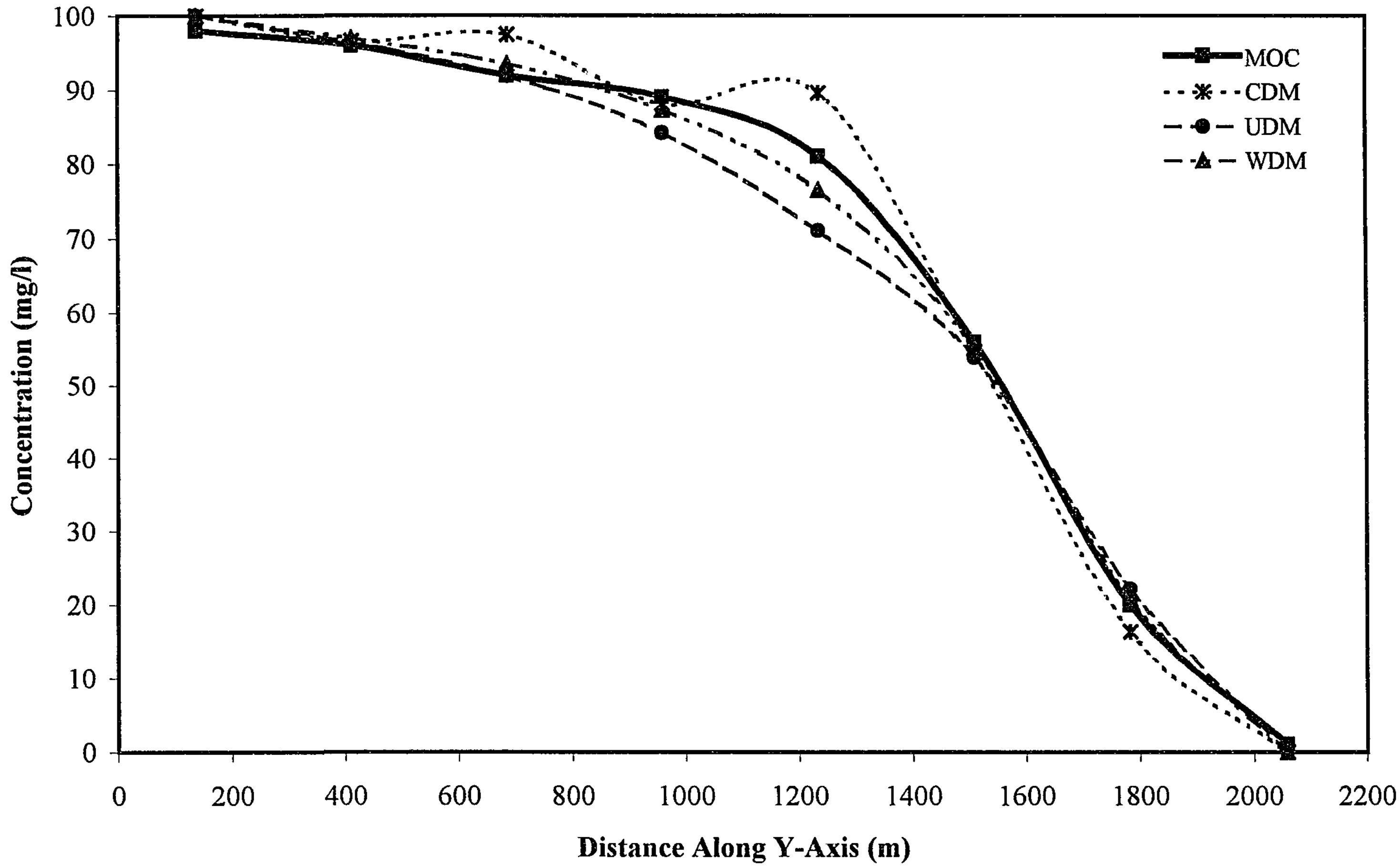


FIG 4.17: COMPARISON OF CONCENTRATION DISTRIBUTION OBTAINED USING CENTRAL, UPWIND, AND WEIGHTED DIFFERENCE WITH MOC SOLUTION ALONG A LINE PARALLEL TO Y AXIS

4.5 VERIFICATION OF SOLUTE TRANSPORT COMPONENT OF STREAMS

The finite difference equations of the linear one-dimensional partial differential equation for an advective nondispersive stream with source term and first order reaction given in Eq. 3.9.2 is embedded in the optimization model as a strict equality constraints. The optimum solution is obtained only after satisfying these constraints.

4.5.1 Check for Mass Balance

As an internal running check the stream mass balance is printed for each time step, and the same obtained for the model application problem discussed in Section 5.1.4.1 is reproduced here as Table 4.5.1. In the table Σ(Mass In) is the sum of upstream (U/S) inflow times U/S concentration (expressed in Tons/day) and waste flow input times waste disposal concentration (in Tons/d), similarly Σ(Mass Out) is the sum of downstream (D/S) outflow times reach concentration and diversion rate times reach concentration. Only for presentation purposes the percent error is calculated here as (ΣMass In - ΣMass Out) divided by ΣMass In times 100. As in the flow model the stream mass balance equations (Eq. 3.9.2) are modeled as strict equality constraints. The optimum solution obtained satsfy these equality constraints.

Table 4.5.1

Streamflow Solute Transport Mass Balance (24th time step)

Reach #	U/S conc. mg/l	D/S conc. mg/l	U/S M_{IN} Tons/d	D/S M_{OUT} Tons/d	Mass Diverted Tons/d	Waste load Input Tons/d	$\sum M_{IN} - \sum M_{OUT}$ Tons/d	Error %
1	1.000	1.0045	35.62	35.78	0.00	0.00	-0.16	-0.45
2	1.004	1.0079	35.78	35.90	0.00	0.00	-0.12	-0.34
3	1.007	1.0102	35.90	35.99	0.00	0.00	-0.09	-0.25
4	1.010	1.0119	35.99	36.05	0.00	0.00	-0.06	-0.17
5	1.011	1.0131	36.05	36.09	0.00	0.00	-0.04	-0.11
6	1.013	1.0140	36.09	36.12	0.00	0.00	-0.03	-0.08
7	1.014	1.0151	36.12	35.96	0.20	0.00	0.16	0.44
8	1.015	1.0159	35.96	35.99	0.00	0.00	-0.03	-0.08
9	1.015	1.0174	35.99	36.04	0.00	0.00	-0.05	-0.14
10	1.017	1.0184	36.04	36.07	0.00	0.00	-0.03	-0.08
11	1.018	1.0170	36.07	36.02	0.00	0.00	0.05	0.14
12	1.017	5.6836	36.02	201.61	0.00	166.3	0.71	0.35
13	5.683	5.6817	201.61	201.54	0.00	0.00	0.07	0.03
14	5.681	5.6814	201.54	201.53	0.00	0.00	0.01	0.00
15	5.681	5.6808	201.53	201.51	0.00	0.00	0.02	0.01
16	5.680	5.6798	201.51	201.47	0.00	0.00	0.04	0.02
17	5.679	5.6750	201.47	201.30	0.00	0.00	0.17	0.08

4.6 VERIFICATION OF THE MANAGEMENT MODEL COMPONENT

The non-linear optimization program (NEWSUMT-A) used in this research work is well tested and is currently used in several ODU research projects by the Mechanical Engineering Department with NASA. As a verification of this model component, the optimum solution obtained using NEWSUMT-A is compared with the optimum solution obtained using SIMPLEX for the case of aquifer management problem, wherein the linear objective function is subjected to a set of linear constraints.

To test the model a 6000 m x 6000 m aquifer is considered. The aquifer is discretized by a constant grid spacing of 600 m. Two potential pumping wells at (3,6) and (6,7) are identified. The no flow boundaries are defined on three sides. On the top boundary a constant head equal to 50 m is specified. Initial piezometric surface of 50 m is defined throughout the aquifer. The aquifer has a constant thickness of 20 m. The hydraulic conductivity is a constant in both directions and equal to 50 m/d. The storage coefficient of the confined aquifer is 0.0005 and the length of the time step is set at 30 d. The management constraints imposed are maximum drawdown of 10 m at any well location in any time step. Maximum pumping capacity of 20000 m^3/d for each well in each time step, and minimum water demand of 10000 m^3/d for each time step are specified.

The management model was solved using NEWSUMT-A routine and by SIMPLEX. The optimum solution obtained for 5 time steps using NEWSUMT-A and SIMPLEX is shown in Table 4.6.1. As can be seen in the table, there is a very close agreement between the two solutions.

Table 4.6.1

Comparison of Optimum Solution Obtained Using NEWSUMT-A and SIMPLEX

Description	Time Steps				
	1	2	3	4	5
OPTIMUM SOLUTION OBTAINED USING NEWSUMT-A					
Objective Function	119886.67				
Well #1 Discharges m^3/d	16993.2	16379.6	16341.8	16339.4	16340.3
Well #2 Discharges m^3/d	8651.3	7289.1	7187.0	7181.2	7183.3
Total m^3/d	25644.6	23668.7	23528.8	23520.9	23523.6
OPTIMUM SOLUTION OBTAINED USING SIMPLEX					
Objective Function	119931.67				
Well #1 Discharges m^3/d	16998.1	16384.2	16346.4	16344.4	16344.9
Well #2 Discharges m^3/d	8656.2	7293.4	7191.3	7185.4	7187.0
Total m^3/d	25654.3	23677.6	23537.7	23529.8	23531.9
Discrepancy (%)	0.038%	0.038%	0.038%	0.038%	0.035%

5. MODEL APPLICATION

The model application presented in this section is aimed at illustrating the prospects of utilizing the comprehensive conjunctive-use management model for water quality and quantity in connected surface water groundwater systems using stochastic inputs and uncertainties.

5.1 MODEL DESCRIPTION

To demonstrate the various features built into the model and its application to a real physical system requires exhaustive data collection efforts from the field, and among users affected by aquifer drawdowns, surface water diversions, quality of groundwater and surface water together with all major consumers which may include municipalities, private and public industries in the region. During this research work no field experiments were conducted to collect all the needed information.

Here, a hypothetical model is constructed based on a real physical system presented in the USGS Water-Resources Investigations Report (87-4240) on the Southeastern Virginia groundwater flow system. Most of the data used in this section regarding hydrogeologic parameters, streamflow characteristics, boundaries of the aquifer, and location of major pumping centers pertains to Yorktown-Eastover aquifer, extracted from the above mentioned USGS Report (87-4240).

Fig 5.1 shows the two dimensional variable finite difference grid configuration (minimum of 300 m to maximum of 600 m on any one side) is superimposed over the model area. The spatial discretization shown incorporates the physical limits of the aquifer. The grid is composed of 34 rows by 41 columns, totalling 1394 cells. Of these cells, 143 are inactive. The left and right boundaries are considered as no-flow boundaries. A constant head of 14.8 m and 13.8 m is specified at the top and bottom boundaries, respectively. Surface water and groundwater are assumed to be in equilibrium to begin with. Based on the boundary conditions the model determined the steady state initial piezometric surface which is used as the initial condition of the aquifer. The model input data file is given in Appendix A5.

To demonstrate various features of the model developed two different scenarios are considered. Both applications demonstrate management of groundwater flow and transport. In the first application a single realization of hydrogeologic parameter field is generated for conjunctive-use management of groundwater flow and transport along with streamflows and solute transport in streams. In the second application multiple realizations of hydrogeologic parameter fields are generated for management of groundwater flow and transport. In particular, the model applications presented here demonstrate many useful features developed such as stochastic inputs and uncertainties with respect to governing flow parameters, variable finite difference grid representation, leaky aquifer, induced infiltration, unit-response matrix generation for aquifer flow and transport, streamflow, solute transport in streams, and conjunctive-use management for water quality and quantity.

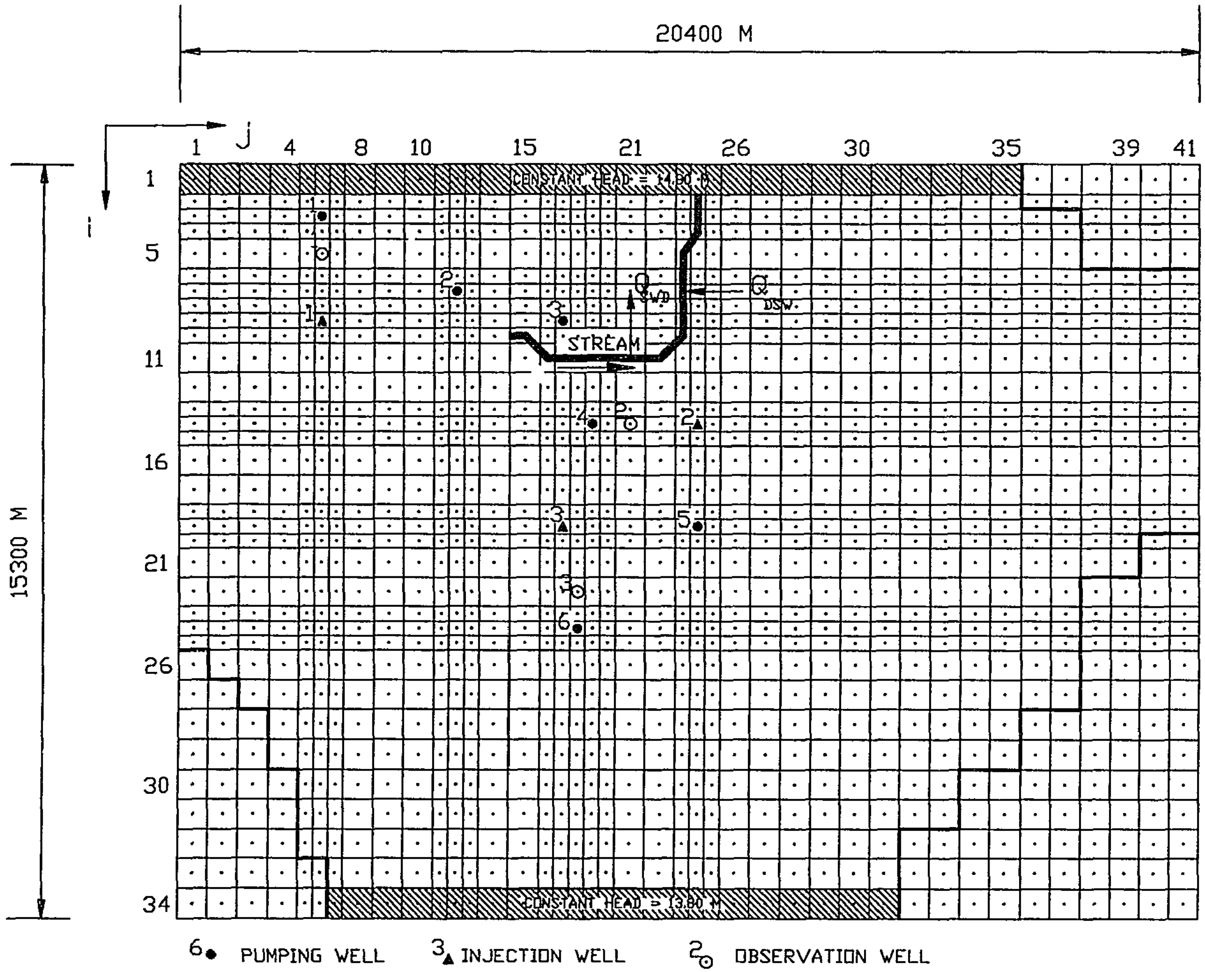


FIG 5.1: FINITE DIFFERENCE GRID CONFIGURATION SHOWING LOCATIONS OF PUMPING WELLS, INJECTION WELLS, STREAM REACHES, AND BOUNDARIES OF AQUIFER

5.1.1 Stochastic Generation of Aquifer Parameters for the Model

Groundwater flow is controlled by hydraulic conductivity and storage coefficient of the confined aquifer overlain by a leaky aquitard. The confined aquifer has a constant thickness of 16.58 m. The confining unit has a constant thickness of 6.1 m and a vertical conductivity of 8.64 x 10^{-6} m/d.

Four hydrogeologic parameters viz permeabilities in X and Y direction (K_x and K_y (m/d)), and confined and unconfined storage coefficients (S_c and S_u) are assumed to be measured at each of the measurement well. The mean of measured data is the same as given in the USGS report (87-4240). The aquifer is divided into four regions. Fig 5.2 shows the regionalization, and location of all measurement wells in the aquifer. The total number of measurement wells in each region varies. The location of the measurement wells in a region and its analysis are discussed separately for each region. The upper and lower bound for the correlation length scale is set as 2100 m $\leq \lambda_x \leq$ 7200 m, and 1800 m $\leq \lambda_y \leq$ 4500 m. The upper and lower bound was selected based on the minimum and maximum distance between the measurement wells in any region.

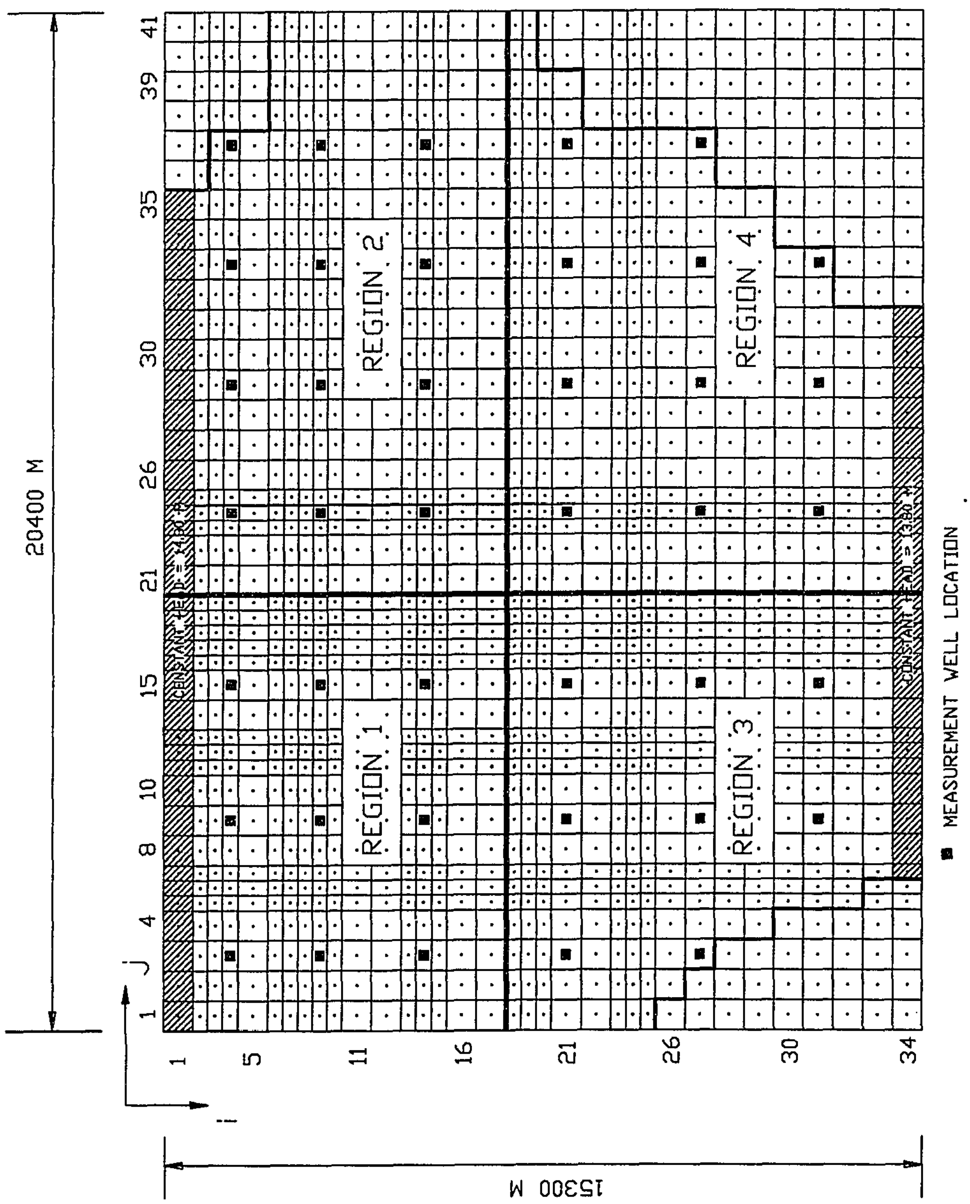


FIG 5.2: REGIONALIZATION AND LOCATION OF MEASUREMENT WELLS

5.1.1.1 Region 1

A total of nine measurement wells are located in Region 1. The location and measurement data are tabulated in Table 5.1.1. Using the measurement data optimum structural parameters are found and is tabulated in Table 5.1.2. Mean and variance given in Table 5.1.2 are the logarithmic values of the random field.

Table 5.1.1

Region 1, Assumed Measurement Data of Hydrogeologic Parameters

Sr No	Row	Col	K_x	K_y	S_c	S_u
1	4	3	4.3	4.3	6.4E-06	1.1E-01
2	4	9	5.1	4.9	8.0E-06	1.3E-01
3	4	15	5.3	5.3	7.0E-06	1.9E-01
4	9	3	4.1	4.1	7.2E-06	1.6E-01
5	9	9	4.5	4.5	8.0E-06	1.0E-01
6	9	15	4.5	4.5	6.5E-06	1.3E-01
7	14	3	4.1	4.1	7.2E-06	2.5E-01
8	14	9	4.4	4.4	7.3E-06	1.8E-01
9	14	15	5.2	5.0	7.0E-06	1.5E-01

Table 5.1.2

Region 1, Optimum Values of MLE Parameters

	K_x	K_y	S_c	S_u
μ	1.53098	1.52423	-11.86155	-1.83902
σ^2	0.00961	0.00837	0.00509	0.07660
λ_x	2437.4	3417.0	2100.0	2626.5
λ_y	1859.9	2539.5	2706.4	1800.0

5.1.1.2 Region 2

A total of twelve measurement wells are located in Region 2. The location and measurement data are tabulated in Table 5.1.3. Using the measurement data optimum structural parameters are found and is tabulated in Table 5.1.4.

Table 5.1.3

Region 2, Assumed Measurement Data of Hydrogeologic Parameters

Sr No	Row	Col	K_x	K_y	S_c	S_u
1	4	24	4.2	4.4	8.4E-06	1.8E-01
2	4	29	5.4	5.4	7.9E-06	1.9E-01
3	4	33	4.8	4.8	7.3E-06	1.8E-01
4	4	37	6.6	6.8	6.7E-06	1.5E-01
5	9	24	4.5	4.5	7.5E-06	2.0E-01
6	9	29	4.9	4.9	7.1E-06	1.7E-01
7	9	33	4.4	4.3	7.0E-06	1.3E-01
8	9	37	5.8	6.0	6.9E-06	1.2E-01
9	14	24	3.9	3.9	7.3E-06	1.5E-01
10	14	29	4.5	4.5	5.3E-06	1.1E-01
11	14	33	3.4	3.4	5.7E-06	1.6E-01
12	14	37	3.6	3.6	7.5E-06	1.3E-01

Table 5.1.4

Region 2, Optimum Values of MLE Parameters

	K_x	K_y	S_c	S_u
μ	1.51085	1.52103	-11.85553	-1.87619
σ^2	0.03747	0.04174	0.01607	0.03451
λ_x	2382.9	2389.1	2631.9	2507.2
λ_y	2176.6	2487.9	1842.4	1800.0

5.1.1.3 Region 3

A total of eight measurement wells are located in Region 3. The location and measurement data are tabulated in Table 5.1.5. Using the measurement data optimum structural parameters found and is tabulated in Table 5.1.6.

Table 5.1.5

Region 3, Assumed Measurement Data of Hydrogeologic Parameters

Sr No	Row	Col	K_x	K_y	S_c	S_u
1	21	3	4.1	3.9	6.2E-06	1.3E-01
2	21	9	4.4	4.4	6.4E-06	1.5E-01
3	21	15	4.9	4.9	6.8E-06	1.8E-01
4	27	3	4.4	4.4	6.6E-06	1.0E-01
5	27	9	4.7	4.6	8.2E-06	1.5E-01
6	27	15	5.1	4.9	7.4E-06	2.1E-01
7	31	9	4.3	4.3	8.5E-06	1.8E-01
8	31	15	4.4	4.4	7.6E-06	1.5E-01

Table 5.1.6

Region 3, Optimum Values of MLE Parameters

	K_x	K_y	S_c	S_u
μ	1.50283	1.48769	-11.86762	-1.89953
σ^2	0.00510	0.00517	0.01283	0.04540
λ_x	3167.9	2293.8	3058.7	2100.0
λ_y	1932.7	2503.5	3433.2	3127.7

5.1.1.4 Region 4

A total of eleven measurement wells are located in Region 4. The location and measurement data are tabulated in Table 5.1.7. Using the measurement data optimum structural parameters are found and is tabulated in Table 5.1.8.

Table 5.1.7

Region 4, Assumed Measurement Data of Hydrogeologic Parameters

Sr No	Row	Col	K_x	K_y	S_c	S_u
1	21	24	4.9	4.9	8.0E-06	1.7E-01
2	21	29	5.0	5.0	6.7E-06	1.9E-01
3	21	33	4.7	4.7	7.3E-06	1.6E-01
4	21	37	4.5	4.5	7.4E-06	1.4E-01
5	27	24	4.8	4.8	7.5E-06	1.8E-01
6	27	29	4.4	4.4	7.0E-06	1.3E-01
7	27	33	3.8	4.5	7.0E-06	1.7E-01
8	27	37	4.1	4.4	7.2E-06	1.2E-01
9	31	24	5.3	5.3	7.0E-06	1.8E-01
10	31	29	4.4	4.4	6.3E-06	1.4E-01
11	31	33	4.2	4.2	6.1E-06	1.3E-01

Table 5.1.8

Region 4, Optimum Values of MLE Parameters

	K_x	K_y	S_c	S_u
μ	1.53881	1.54328	-11.85947	-1.87394
σ^2	0.00958	0.00482	0.00604	0.02439
λ_x	4374.1	2374.3	2361.0	2100.0
λ_y	3230.2	3482.7	2715.4	2577.1

5.1.1.5 Gaussian Conditional Simulation

The optimum structural parameters obtained for each region is used in generating maps of random hydrogeologic parameter fields by the Gaussian conditional simulation approach. Fig 5.3 to Fig 5.6 show these maps for a single realization of the aquifer parameters.

5.1.2 Conjunctive-Use Management of Water Quantity in the Connected Surface Water Groundwater System

The aquifer simulation program developed is used in obtaining the unit-response matrix for the six potential pumping wells, three injection wells, and seventeen stream reaches. A constant waste injection discharge rate of 1000 m^3/d is specified at the injection wells. A unit-discharge rate of 1000 m^3/d is used in developing the unit-response matrix. The objective is to maximize the pumping from groundwater wells and to maximize diversions from the surface water. This is described by the Eq. 3.10.1.

5.1.2.1 Modeling Stream

The mean annual stream flow rates were used in describing the stream inflow hydrograph. This is constant and equal to 3.5622×10^7 m^3/d. The stream is modeled as a wide rectangular channel of constant top width equal to 100 m, the stream bed has a uniform slope of 1.0×10^{-6} m/m, the Manning's roughness coefficient equal to 0.04, thickness of the stream bed equal to 0.3048 m, with a vertical conductivity of 0.0001905 m/d, and the stream bed penetrates the confined aquifer. Reach 7 is identified as a potential diversion site, while reach 12 is identified as a potential waste disposal site,

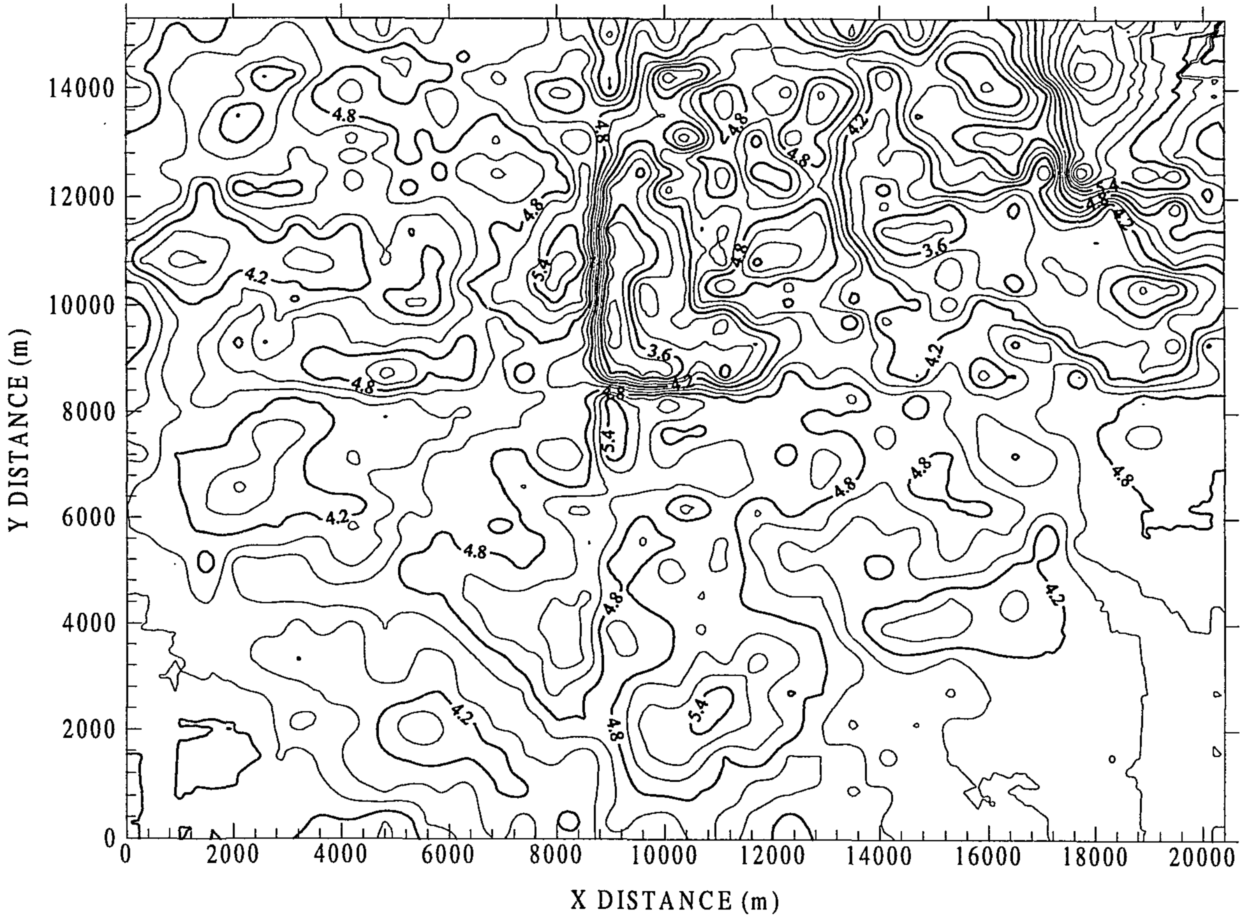


FIG 5.3: MAP OF HYDRAULIC CONDUCTIVITY (m/d) IN X DIRECTION

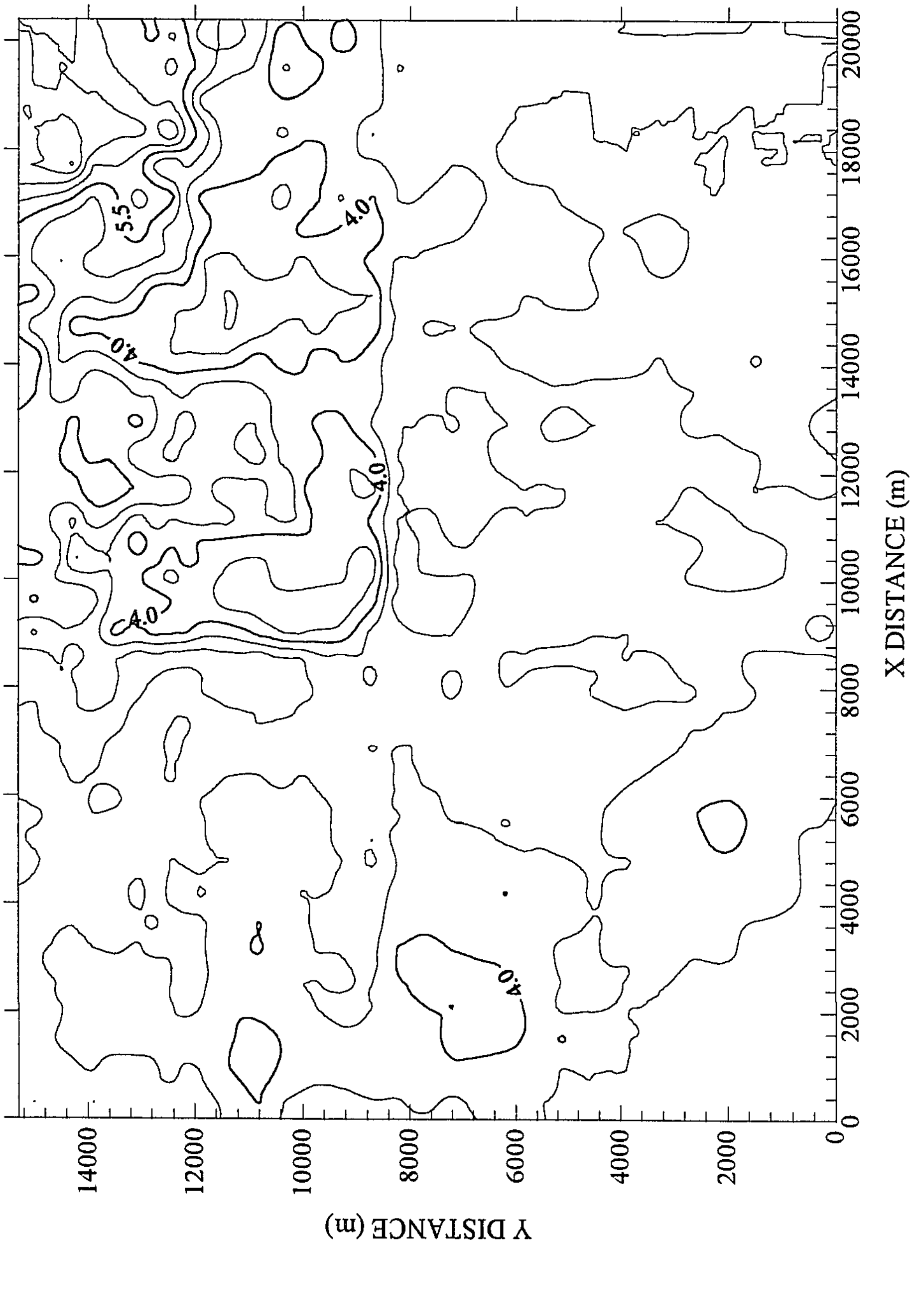


FIG 5.4: MAP OF HYDRAULIC CONDUCTIVITY (m/d) IN Y DIRECTION

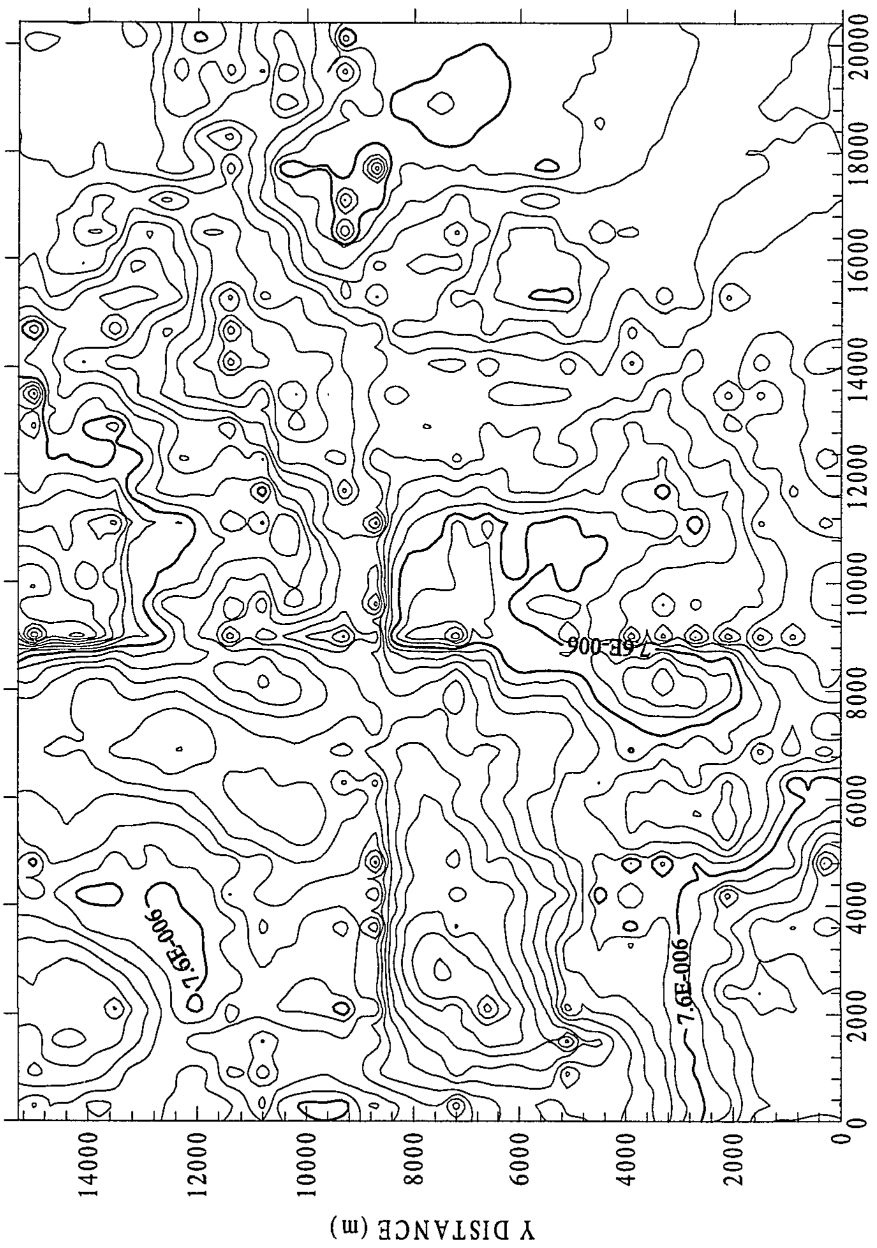


FIG 5.5: MAP OF CONFINED AQUIFER STORAGE COEFFICIENT

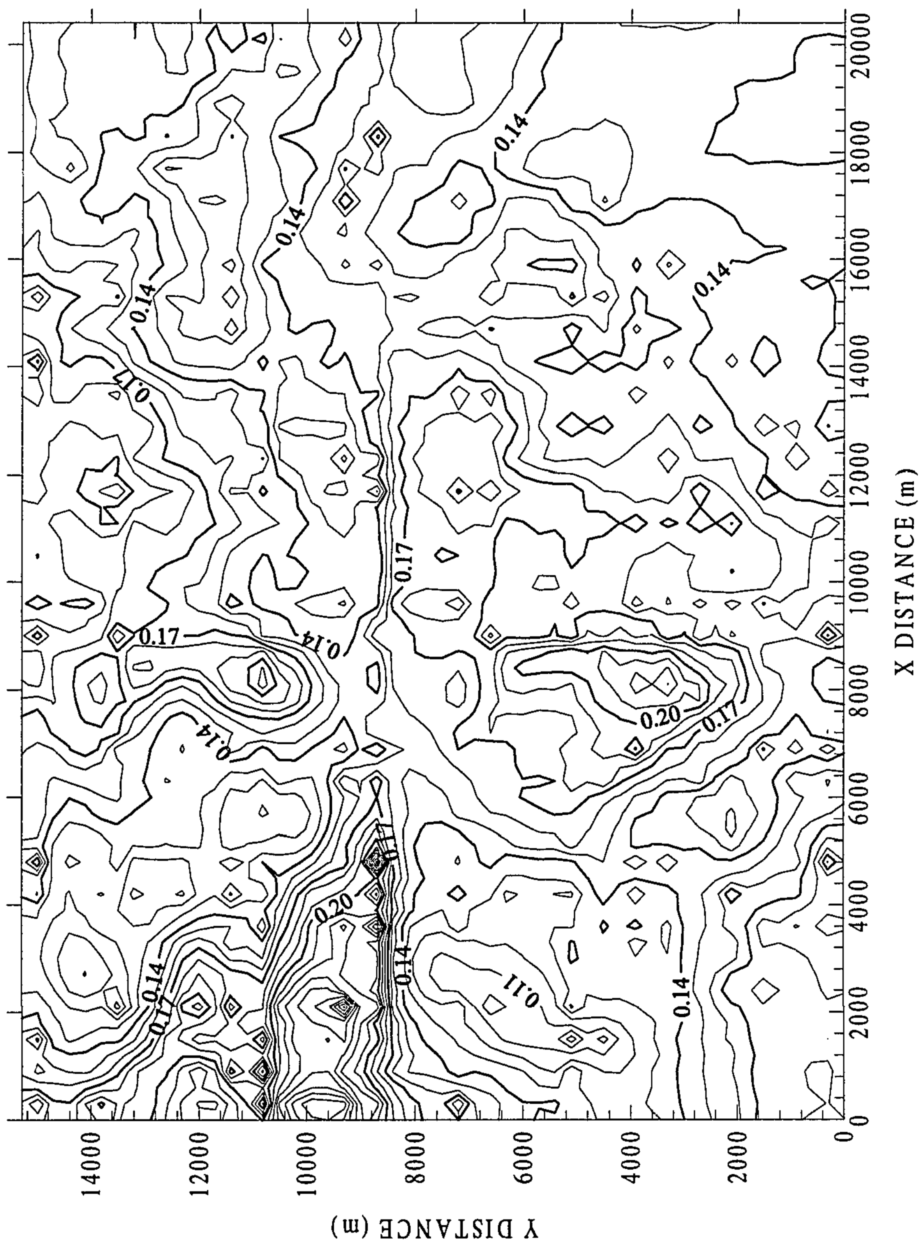


FIG 5.6: MAP OF UNCONFINED AQUIFER STORAGE COEFFICIENT

the locations of these are shown in Fig 5.1. A constant waste disposal discharge rate of 50000 m^3/d is specified.

5.1.2.2 Modeling System and Management Constraints

Eq. 3.10.2 to Eq. 3.10.4 were used in describing the system constraints. The management and system capacity constraints described in Eq. 3.10.5 to Eq. 3.10.10 were used with the imposed constraint values as tabulated in Table 5.1.9.

Table 5.1.9

Constraints Used in Describing the Quantity Management Model

Description	Eq. No	Name	Type	Value
Limit on Aquifer Drawdowns	3.10.5	$s^*(k,NT)$	$\leq$	Variable. Ranges from 4.0 m to 10.0 m
Maintenance of minimum stream depth	3.10.6	$Y_R^*(i)$	$\geq$	20.0 m
Minimum water demands to be satisfied	3.10.7	$D^*(i)$	$\geq$	200000 m^3/d
Minimum groundwater pumping required	3.10.8	$D_w^*(i)$	$\geq$	Variable. Ranges from 3000 to 6000 m^3/d
Cap on the pumping capacity	3.10.9	$Q_w^{max}(j,i$	$\leq$	3000 m^3/d
Cap on surface water diversion	3.10.10	$Q_{SWD}^{max}(j,i$	$\leq$	200000 m^3/d

The control parameters for the conjunctive-use optimization of water quantities are described in Table 5.1.10.

Table 5.1.10

Control Parameters for the Conjunctive-Use Management Model - Quantity

Description	Name	Value
Total number of decision variables	NDV	984
Total number of constraints	NTCE	1273
Number of non-linear equality constraints	NLEQ	782
Number of linear equality constraints	LEQ	35
Number of linear inequality constraints	LIEQ	456

5.1.2.3 Optimization of Water Quantity

The conjunctive-use management model framed above was solved using the available NEWSUMT-A non-linear optimization program. The output of optimum groundwater pumping quantities and surface water diversion rates is reproduced here as Table 5.1.11.

5.1.3 Discussion of Results for Conjunctive-Use Management of Water Quantity

The plot of aquifer heads for the optimum solution at the end of 24^{th} time step (after 7200 days) is shown in Fig 5.7. The plot of river heads for optimum solution of surface water diversions at the end of 24^{th} time step is shown in Fig 5.8. Note that the sudden drop in river head at around 2000 m is due to surface water diversions in reach 7, and the gain in river head at around 4100 m is due to wastewater disposal in reach 12.

Table 5.1.11

Optimum Well Discharges and Surface Water Diversions

			WELL DISCHARGES AND SURFACE WATER DIVERSIONS IN CUBIC METERS PER DAY											
Well	LOCATION		TIME STEPS											
#	IW	JW	1	2	3	4	5	6	7	8	9	10	11	12
1	3	6	569.4	582.5	620.2	635.7	804.4	822.0	848.3	865.9	1043.5	1062.3	1088.0	1108.1
2	7	12	465.8	476.1	491.8	509.0	627.8	637.7	650.9	664.9	795.4	805.6	819.5	834.0
3	9	17	440.4	465.0	456.6	506.4	610.4	633.5	643.3	676.1	795.4	817.7	830.8	862.5
4	14	19	619.0	624.3	592.9	633.7	742.0	750.5	741.8	758.1	878.9	883.4	873.1	878.5
5	19	24	568.5	564.4	576.4	580.5	694.7	695.5	701.6	703.1	825.7	826.1	832.3	832.2
6	24	18	517.9	516.7	535.0	535.0	653.4	653.0	659.0	655.8	787.7	780.0	774.7	757.7
Total GW Pumping			3181	3229	3273	3400	4133	4192	4245	4324	5127	5175	5218	5273
Min Pumping Required			3000	3000	3000	3000	4000	4000	4000	4000	5000	5000	5000	5000
Reach		7	38	199900	199956	199910	199789	199895	199787	199868	199602	199677	199614	199672
Total of GW + SW			3219	203129	203229	203310	203921	204088	204032	204192	204729	204852	204833	204945
Total Demand to be met			3000	200000	200000	200000	200000	200000	200000	200000	200000	200000	200000	200000

			WELL DISCHARGES AND SURFACE WATER DIVERSIONS IN CUBIC METERS PER DAY											
Well	LOCATION		TIME STEPS											
#	IW	JW	13	14	15	16	17	18	19	20	21	22	23	24
1	3	6	1296.0	1295.3	1296.1	1295.4	1295.9	1295.6	1295.9	1295.5	1296.0	1295.4	1295.2	1298.9
2	7	12	975.0	974.5	974.8	974.6	974.8	974.7	974.7	974.6	974.6	974.6	974.5	975.9
3	9	17	992.7	994.9	992.9	994.1	993.4	993.9	993.3	994.1	993.0	994.0	994.3	985.4
4	14	19	1012.0	1013.7	1011.7	1013.2	1012.0	1012.8	1012.2	1012.9	1011.8	1012.8	1013.3	1005.1
5	19	24	967.4	966.5	967.4	967.1	967.0	966.9	967.3	966.9	967.4	967.0	967.0	970.6
6	24	18	867.8	866.6	867.9	867.1	867.8	867.4	867.8	867.4	868.0	867.7	867.6	872.4
Total GW Pumping			6111	6112	6111	6112	6111	6111	6111	6111	6111	6112	6112	6108
Min Pumping Required			6000	6000	6000	6000	6000	6000	6000	6000	6000	6000	6000	6000
Reach		7	199420	199494	199430	199500	199429	199512	199412	199524	199391	199546	199363	199694
Total of GW + SW			205531	205606	205541	205611	205540	205623	205523	205635	205502	205658	205475	205802
Total Demand to be met			200000	200000	200000	200000	200000	200000	200000	200000	200000	200000	200000	200000

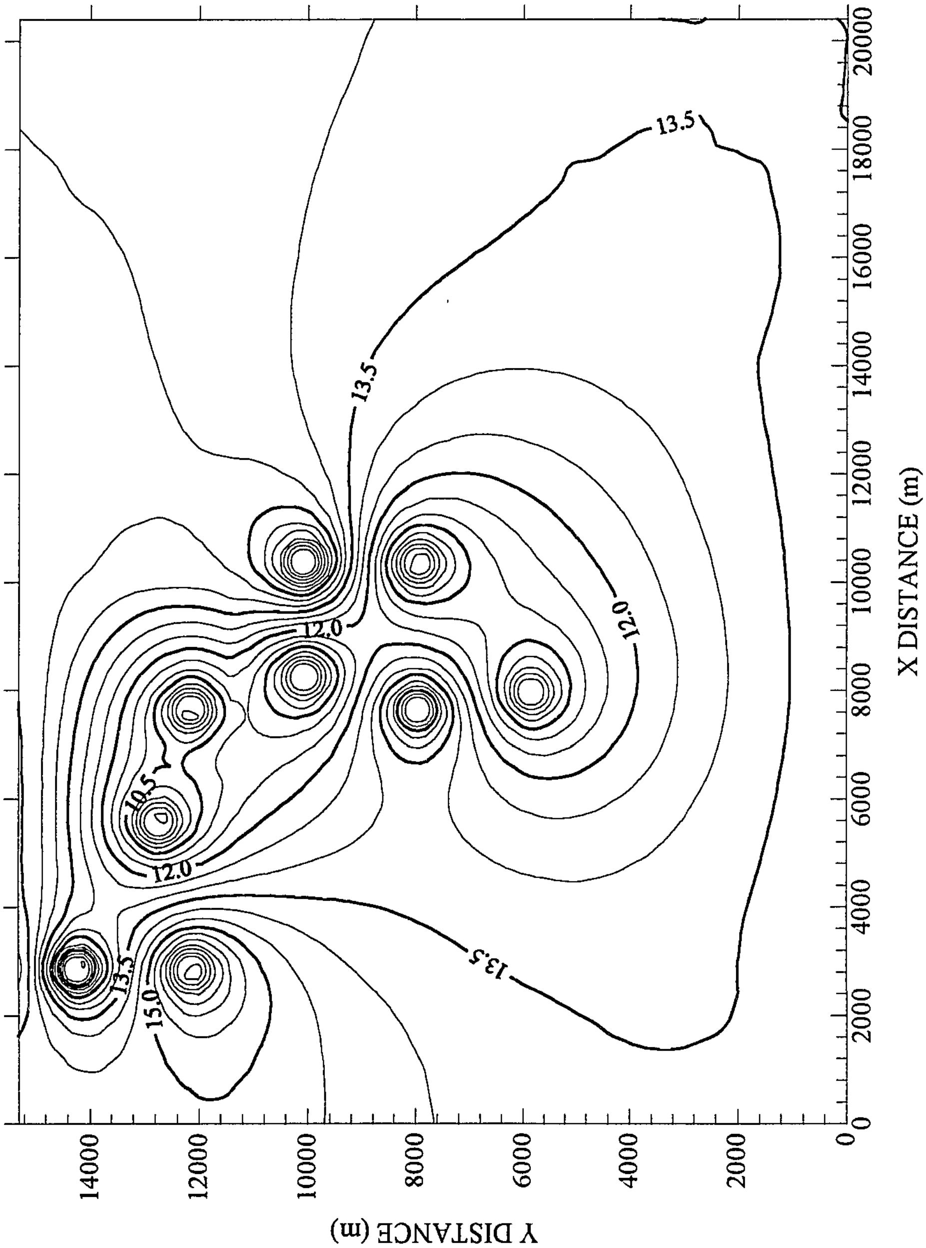


FIG 5.7: MAP OF AQUIFER HEADS (m) FOR OPTIMAL WELL PUMPING

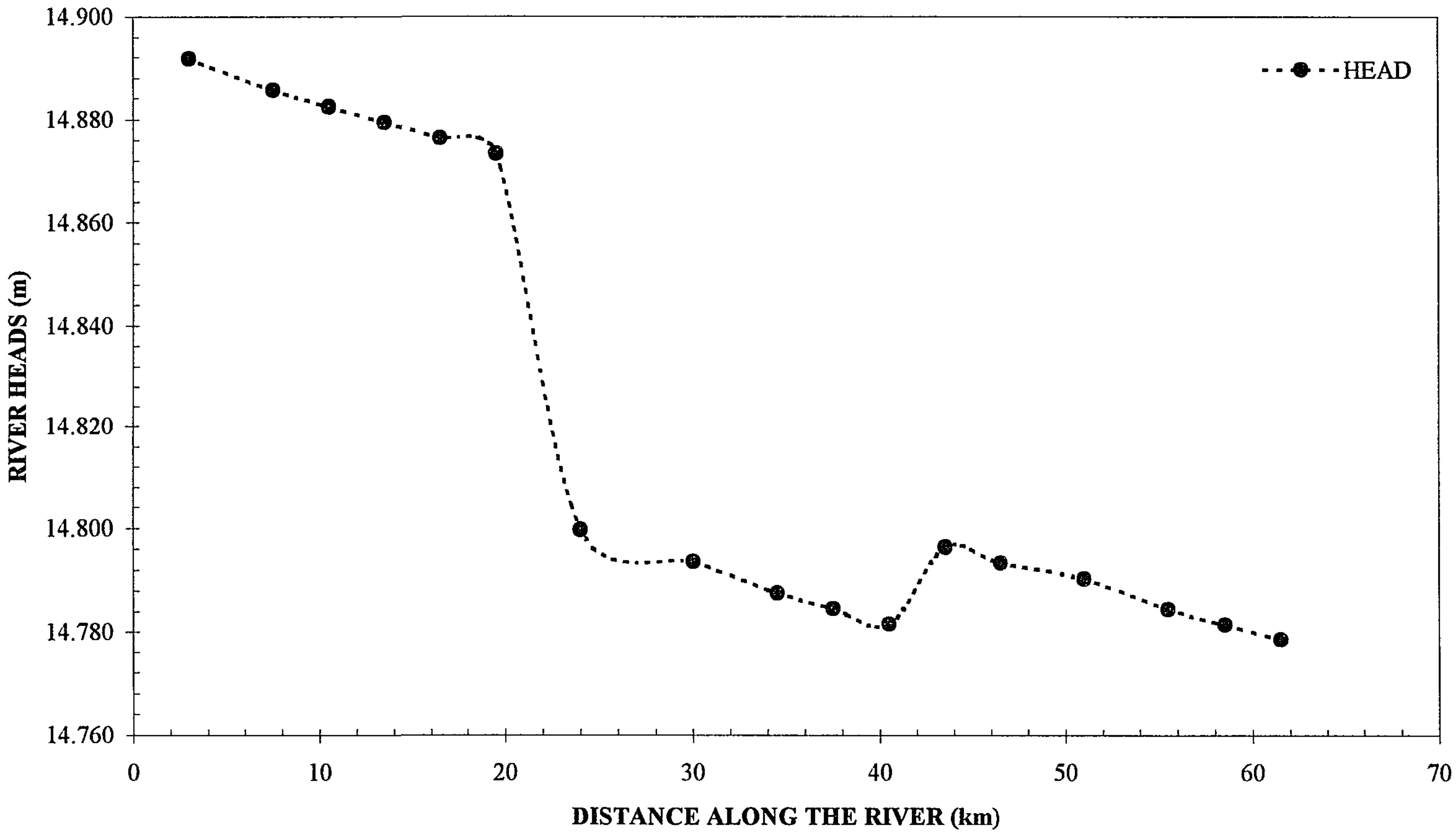


FIG 5.8: PLOT OF RIVER HEADS FOR OPTIMUM SURFACE WATER DIVERSION

The optimum solution obtained did satisfy all the system and management constraints. The output of streamflow mass balance at the end of 24th time step is reproduced here as Table 5.1.12. As seen in the table the induced infiltration rates from or to the surface water is less significant, because the nearest groundwater pumping well to the stream is more than 750 m.

Table 5.1.12

Streamflow Mass Balance (24th time step)

Reach #	Stream Depth (m)	U/S Qin (1000 m^3/d)	D/S Qout (1000 m^3/d)	Diversion (1000 m^3/d)	Infiltration (m^3/d)	Waste flow Input(1000 m^3/d)	Σ Qin - Σ Qout (m^3/d)	Error %
1	21.0916	35622.0	35621.8	0.0	-150.	0.0	4.	0.00
2	21.0916	35621.8	35621.8	0.0	-76.	0.0	-16.	0.00
3	21.0916	35621.8	35621.7	0.0	-77.	0.0	-12.	0.00
4	21.0915	35621.7	35621.7	0.0	-72.	0.0	-4.	0.00
5	21.0915	35621.7	35621.6	0.0	-65.	0.0	-4.	0.00
6	21.0915	35621.6	35621.5	0.0	-56.	0.0	-4.	0.00
7	21.0206	35621.5	35421.8	199.7	-77.	0.0	-45.	0.00
8	21.0206	35421.8	35421.8	0.0	-36.	0.0	-8.	0.00
9	21.0206	35421.8	35421.8	0.0	-12.	0.0	-16.	0.00
10	21.0206	35421.8	35421.8	0.0	-13.	0.0	0.	0.00
11	21.0206	35421.8	35421.8	0.0	-13.	0.0	-4.	0.00
12	21.0383	35421.8	35471.8	0.0	-13.	50.0	-4.	0.00
13	21.0383	35471.8	35471.8	0.0	-12.	0.0	0.	0.00
14	21.0383	35471.8	35471.7	0.0	-20.	0.0	0.	0.00
15	21.0383	35471.7	35471.7	0.0	-6.	0.0	4.	0.00
16	21.0383	35471.7	35471.7	0.0	-4.	0.0	-4.	0.00
17	21.0383	35471.7	35471.7	0.0	-3.	0.0	-4.	0.00

The output of check for principle of superposition at the end of 24th time step is reproduced here as Table 5.1.13.

Table 5.1.13

Check for Principle of Superposition (24th time step)

KP	I	J	Total s* (m)	H (m) at KP	Head H** (m)	Error (%)	Remarks
1	3	6	9.0574	5.6994	5.6965	-0.0500	Pump Well #1
2	7	12	8.8864	5.7885	5.7799	-0.1500	Pump Well #2
3	9	17	8.9514	5.6891	5.6776	-0.2000	Pump Well #3
4	14	19	8.5287	6.0012	5.9838	-0.2900	Pump Well #4
5	19	24	8.5831	5.8275	5.8085	-0.3300	Pump Well #5
6	24	18	8.0520	6.2410	6.2222	-0.3000	Pump Well #6
7	10	15	3.6530	10.9717	10.9597	-0.1100	Reach #1
8	11	16	3.5838	11.0165	11.0028	-0.1200	Reach #2
9	11	17	3.6303	10.9698	10.9561	-0.1300	Reach #3
10	11	18	3.4105	11.1896	11.1758	-0.1200	Reach #4
11	11	19	3.0565	11.5439	11.5302	-0.1200	Reach #5
12	11	20	2.6336	11.9673	11.9538	-0.1100	Reach #6
13	11	21	1.8096	12.7924	12.7792	-0.1000	Reach #7
14	11	22	0.7095	13.8934	13.8804	-0.0900	Reach #8
15	10	23	0.3847	14.2432	14.2319	-0.0800	Reach #9
16	9	23	0.4642	14.1798	14.1694	-0.0700	Reach #10
17	8	23	0.4956	14.1653	14.1560	-0.0700	Reach #11
18	7	23	0.5045	14.1735	14.1654	-0.0600	Reach #12
19	6	23	0.4816	14.2131	14.2061	-0.0500	Reach #13
20	5	23	0.4102	14.3092	14.3038	-0.0400	Reach #14
21	4	24	0.2112	14.5319	14.5282	-0.0300	Reach #15
22	3	24	0.1454	14.6153	14.6126	-0.0200	Reach #16
23	2	24	0.0855	14.6919	14.6903	-0.0100	Reach #17
24	5	6	1.8899	12.8250	12.8192	-0.0500	Obs Well #1
25	14	21	3.0226	11.5051	11.4882	-0.1500	Obs Well #2
26	22	18	3.3485	10.9897	10.9702	-0.1800	Obs Well #3

Note : * Indicates the total drawdown computed using the Eq. 3.4.2
: ** Indicates the simulated head using the aquifer simulation program developed.

The water demand specified within each time step is fully satisfied with pumping from groundwater wells and surface water diversions. Also, the minimum groundwater pumping specified is satisfied. The groundwater pumping capacity constraints were found to be redundant due to limitations of aquifer drawdowns set by the management constraints (maximum of 10.0 m). The optimal surface water diversions has reached the upper bound of diversion capacity. The minimum stream depth criterion specified was found to be redundant due to limitations on the diversion capacity imposed.

5.1.4 Conjunctive-Use Management of Water Quality in the Connected Surface Water Groundwater System

The aquifer piezometric heads obtained for optimum solution serves to describe the associated groundwater velocities in the aquifer system. The location of potential injection wells and stream reaches are shown in Fig 5.1. The groundwater solute transport is modeled for a conservative substance (such as NaCl) with decay rate = 0/day. The longitudinal and transverse dispersivities are constant throughout the aquifer and equal to 100 m and 40 m, respectively. The porosity of the aquifer is constant and equal to 0.30. The quadratic upstream interpolation method is used to model the advective transport. A barrier boundary condition is specified on the left and right sides, and a constant concentration of 0 mg/l is specified at the top and bottom boundaries of the aquifer model consistent with the flow model.

The aquifer transport simulation program is used in generating the unit-concentration response matrix for the three potential injection wells, and seventeen stream

reaches. A unit-concentration of 3000 kg/d is used in developing the unit-concentration response matrix. In generating unit-concentration response function 24 simulation runs are required for each potential injection well for the single realization considered here; one simulation for each of 24 time steps specified. To assemble the complete response matrix a total of 480 simulations were required. The objective of the water quality management model is to maximize the waste input concentration through the potential injection wells and the waste disposal concentration into the surface water. The objective function is described in Eq. 3.10.11.

5.1.4.1 Modeling Solute Transport in Streams

The concentration associated with the stream inflow hydrograph is user specified and equal to 1.0 mg/l constant. The solute transport in the stream is modeled for a conservative substance (with decay rate equal to 0/day). The quantity management model simulated transient stream depths, reach inflow, outflow, and storage are used in describing the flow under optimum conditions.

5.1.4.2 Modeling System and Management Constraints for Water Quality

Eq. 3.10.12 and Eq. 3.10.13 are used in describing the system mass balance constraints. The management and system capacity constraints described in Eq. 3.10.14 through 3.10.19 are used with the imposed constraint values as tabulated in Table 5.1.14. The control parameters for optimization are described in Table 5.1.15.

Table 5.1.14

Constraints Used in Describing the Quality Management Model

Description	Eq. No	Name	Type	Value
Limit on groundwater pumping concentration	3.10.14	C_w^* (k,NT)	≤	2.0 mg/l
Limit on aquifer concentration at observation wells (750 m radius from the pumping well)	3.10.14	C_w^* (k,NT)	≤	100 mg/l
Maintenance of minimum stream water quality	3.10.15	$C_R^*(i)$	≤	6.0 mg/l
Minimum waste load demand to be satisfied	3.10.16	$WL^*(i)$	≥	1.75E8 g/d
Minimum groundwater injection required	3.10.17	$WL_{INJ}^*(i)$	≥	Variable. Ranges from 4.0E6 to 1.5E7 g/d
Cap on the injection capacity	3.10.18	$C_w^{\max}(j,i)$	≤	6000 mg/l
Cap on waste disposal into surface water	3.10.19	$C_R^{\max}(j,i)$	≤	10000 mg/l

Table 5.1.15

Control Parameters for the Conjunctive-Use Quality Management Model

Description	Name	Value
Total number of decision variables	NDV	504
Total number of constraints	NTCE	793
Number of linear equality constraints	LEQ	409
Number of linear inequality constraints	LIEQ	384

5.1.4.3 Optimization of Water Quality

Here also, the conjunctive-use management model for water quality framed above was solved using the NEWSUMT-A computer program. The output of groundwater injection rates with optimum concentration and surface water disposal rates with associated optimum surface water disposal concentration is reproduced here as Table 5.1.16.

5.1.5 Discussion of Results for Conjunctive-Use Management of Water Quality

The plot of aquifer concentrations for the optimum solution at the end of 24^{th} time step (after 7200 days) is shown in Fig 5.9. The plot of river concentrations for the optimum solution of surface water disposal at the end of 24^{th} time step (after 7200 days) is shown in Fig 5.10. The waste disposal of concentration into the stream at around 4100 m (in the 12^{th} reach) results in a sudden increase in stream concentration, and this is seen in Fig 5.10.

Table 5.1.16

Optimum Concentration Injection and Waste Disposal Concentration

Inj Well	LOCATION		INJECTION CONCENTRATION AND SURFACE WATER WASTE DISPOSAL CONCENTRATION (mg/l)											
			TIME STEPS											
#	IRW	JRW	1	2	3	4	5	6	7	8	9	10	11	12
1	9	6	1320.8	1554.4	2036.4	2301.0	3059.7	3908.9	4873.2	4936.5	4981.3	5020.2	5064.3	5111.5
2	14	24	1677.3	1536.3	1444.6	1252.5	1124.6	1101.4	1545.9	1744.5	2161.0	2824.7	3873.5	4662.2
3	19	17	5214.9	5230.7	5256.2	5241.5	5227.3	5215.1	5273.1	5254.7	5234.4	5215.9	5203.6	5200.5
Total Injection (Tons/day)			8.2	8.3	8.7	8.8	9.4	10.2	11.7	11.9	12.4	13.1	14.1	15.0
Min Inj Requirement (Tons/d			4.0	4.0	4.0	6.0	6.0	6.0	10.0	10.0	10.0	10.0	10.0	10.0
Reach		12	49.6	3390.5	3365.6	3391.2	3389.4	3395.2	3364.8	3370.3	3365.6	3369.6	3363.8	3371.2
Tot Wasteload (INJ+SW)			8.2	177.8	177.0	178.4	178.9	180.0	179.9	180.5	180.7	181.5	182.3	183.5
Wasteload demand to be met			4.0	175.0	175.0	175.0	175.0	175.0	175.0	175.0	175.0	175.0	175.0	175.0

Inj Well	LOCATION		INJECTION CONCENTRATION AND SURFACE WATER WASTE DISPOSAL CONCENTRATION (mg/l)											
			TIME STEPS											
#	IRW	JRW	13	14	15	16	17	18	19	20	21	22	23	24
1	9	6	5350.5	5356.3	5361.3	5364.5	5366.4	5366.3	5365.2	5362.4	5359.6	5356.2	5354.4	5354.4
2	14	24	5270.1	5298.5	5323.6	5345.0	5363.6	5378.3	5389.6	5395.9	5397.7	5393.5	5383.9	5369.6
3	19	17	5373.1	5366.0	5360.5	5355.6	5352.2	5349.3	5347.8	5346.7	5347.2	5348.0	5350.3	5353.2
Total Injection (Tons/day)			16.0	16.0	16.0	16.1	16.1	16.1	16.1	16.1	16.1	16.1	16.1	16.1
Min Inj Requirement (Tons/d			15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0
Reach		12	3350.0	3365.3	3349.2	3365.9	3347.7	3367.2	3345.7	3369.3	3343.6	3370.8	3343.7	3327.0
Tot Wasteload (INJ+SW)			183.5	184.3	183.5	184.4	183.5	184.5	183.4	184.6	183.3	184.6	183.3	182.4
Wasteload demand to be met			175.0	175.0	175.0	175.0	175.0	175.0	175.0	175.0	175.0	175.0	175.0	175.0

Note: Waste injection recharge rate at each injection well is specified as a constant and equal to 1000 m3/d.
Waste disposal discharge rate into surface water is a constant and equal to 50000 m3/d.
Total Waste Disposal and Wasteload demand are expressed in grams/day.

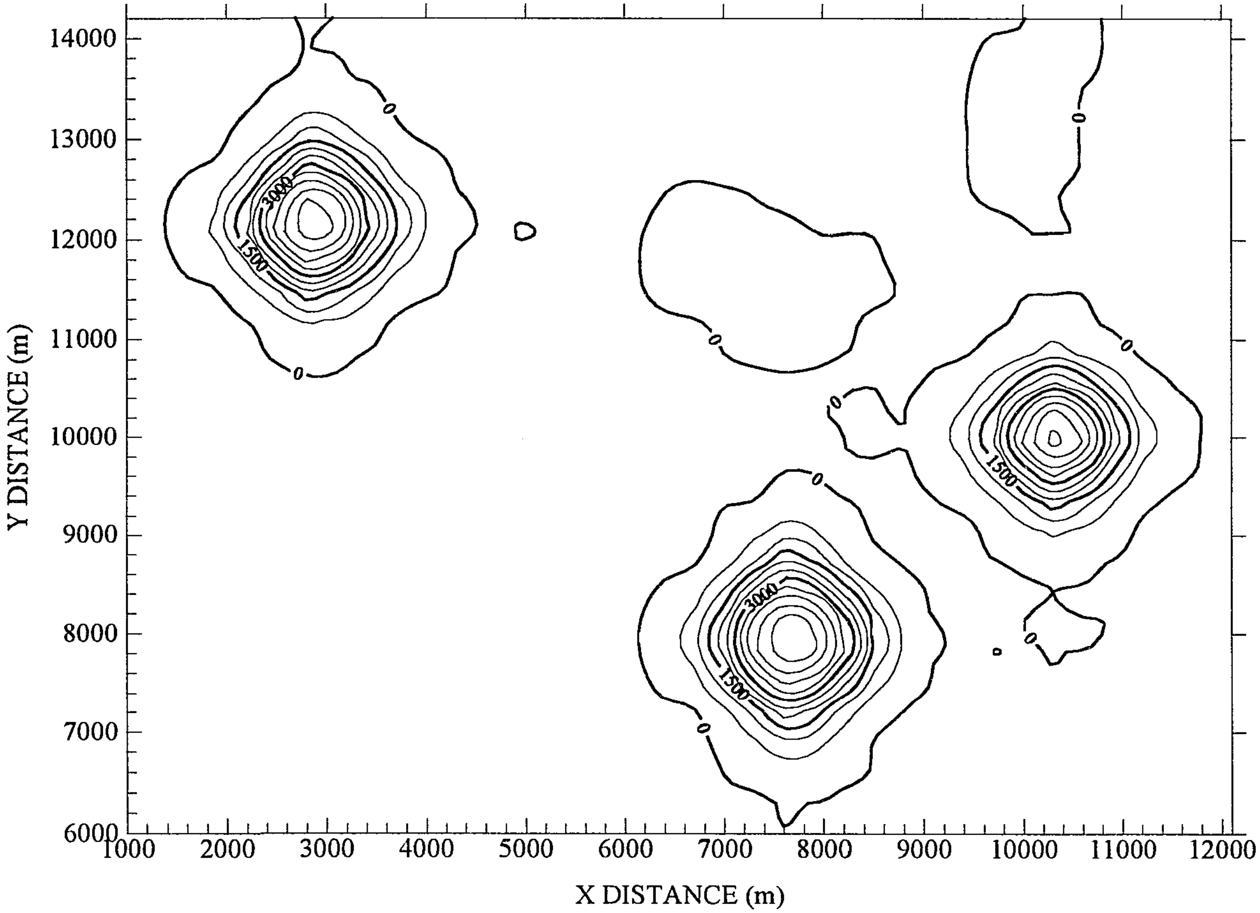


FIG 5.9: MAP OF AQUIFER CONCENTRATION (mg/l) FOR OPTIMUM CONCENTRATION INJECTION

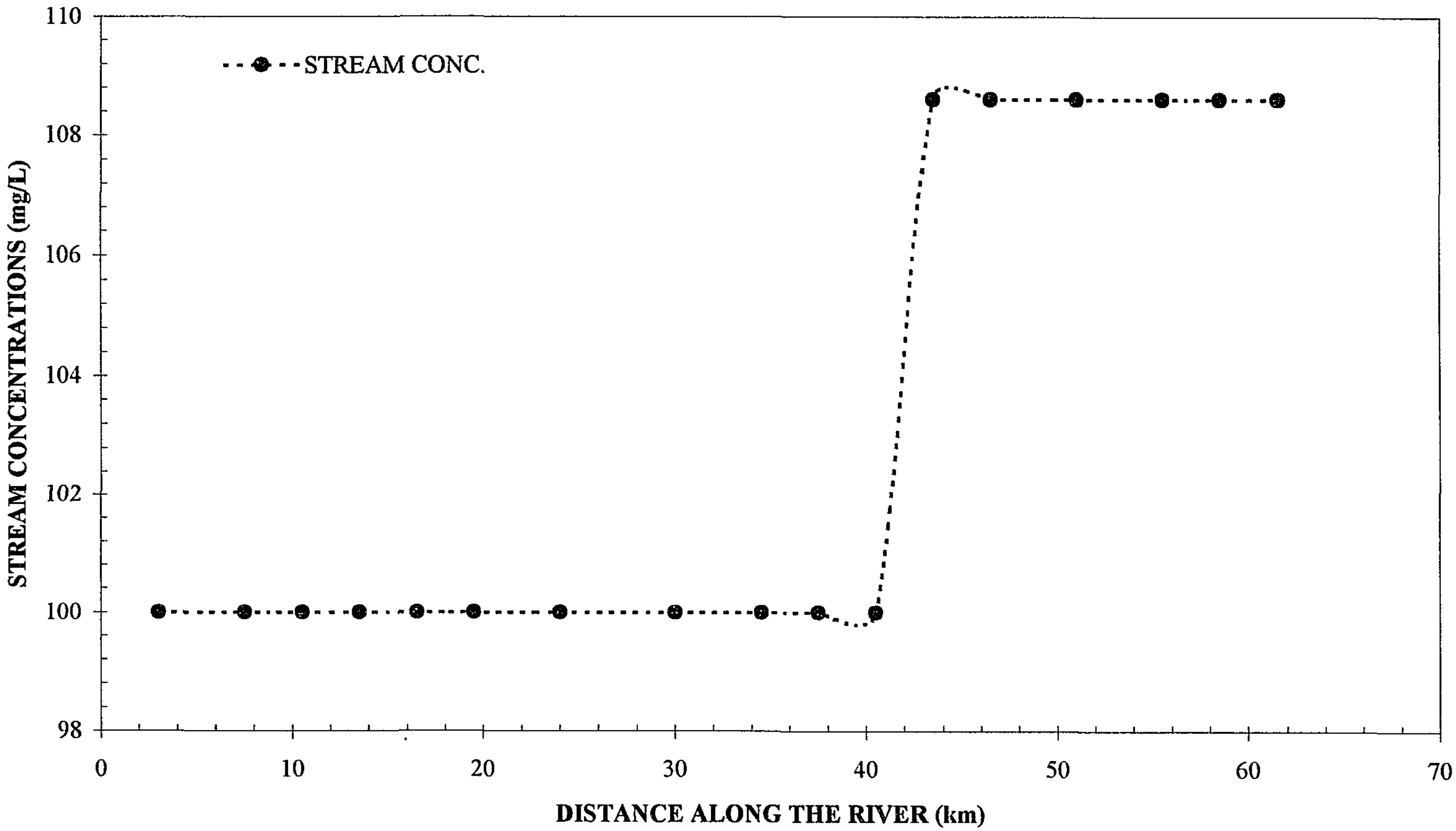


FIG 5.10: PLOT OF STREAM CONCENTRATION FOR OPTIMUM SURFACE WATER DISPOSAL

The optimum solution obtained did satisfy all the system and management constraints. The output of stream solute transport mass balance at the end of 24th time step is reproduced here as Table 5.1.17. The check for superposition is shown in Table 5.1.18.

Table 5.1.17

Streamflow Solute Transport Mass Balance (24th time step)

Reach #	U/S conc. mg/l	D/S conc. mg/l	U/S M_{IN} Tons/d	D/S M_{OUT} Tons/d	Mass Diverted Tons/d	Waste load Input Tons/d	$\sum M_{IN} - \sum M_{OUT}$ Tons/d	Error %
1	1.0000	1.0045	35.62	35.78	0.00	0.00	-0.16	-0.45
2	1.0045	1.0079	35.78	35.90	0.00	0.00	-0.12	-0.34
3	1.0079	1.0102	35.90	35.99	0.00	0.00	-0.09	-0.25
4	1.0102	1.0119	35.99	36.05	0.00	0.00	-0.06	-0.17
5	1.0119	1.0131	36.05	36.09	0.00	0.00	-0.04	-0.11
6	1.0131	1.0140	36.09	36.12	0.00	0.00	-0.03	-0.08
7	1.0140	1.0151	36.12	35.96	0.20	0.00	0.16	0.44
8	1.0151	1.0159	35.96	35.99	0.00	0.00	-0.03	-0.08
9	1.0159	1.0174	35.99	36.04	0.00	0.00	-0.05	-0.14
10	1.0174	1.0184	36.04	36.07	0.00	0.00	-0.03	-0.08
11	1.0184	1.0170	36.07	36.02	0.00	0.00	0.05	0.14
12	1.0170	5.6836	36.02	201.61	0.00	166.3	0.71	0.35
13	5.6836	5.6817	201.61	201.54	0.00	0.00	0.07	0.03
14	5.6817	5.6814	201.54	201.53	0.00	0.00	0.01	0.00
15	5.6814	5.6808	201.53	201.51	0.00	0.00	0.02	0.01
16	5.6808	5.6798	201.51	201.47	0.00	0.00	0.04	0.02
17	5.6798	5.6750	201.47	201.30	0.00	0.00	0.17	0.08

Table 5.1.18

Check for Principle of Superposition (24th time step)

KP	I	J	Total c^* (mg/l)	C (mg/l) at KP	Conc C^{**} (mg/l)	Error (%)	Remarks
1	3	6	-0.0000	0.0000	0.0000	0.0000	Pump Well #1
2	7	12	-0.0009	0.0009	0.0009	0.0000	Pump Well #2
3	9	17	-0.0122	0.0122	0.0122	0.0000	Pump Well #3
4	14	19	-0.0000	0.0000	0.0000	0.0000	Pump Well #4
5	19	24	-0.0000	0.0000	0.0000	0.0000	Pump Well #5
6	24	18	-0.1036	0.1036	0.1036	0.0000	Pump Well #6
7	10	15	-0.7399	0.7399	0.7399	0.0000	Reach #1
8	11	16	-0.4016	0.4016	0.4016	0.0000	Reach #2
9	11	17	-0.4666	0.4666	0.4666	0.0000	Reach #3
10	11	18	-0.3906	0.3906	0.3906	0.0000	Reach #4
11	11	19	-0.3754	0.3754	0.3754	0.0000	Reach #5
12	11	20	-0.3218	0.3218	0.3218	0.0000	Reach #6
13	11	21	-0.2263	0.2263	0.2263	0.0000	Reach #7
14	11	22	-0.0000	0.0000	0.0000	0.0000	Reach #8
15	10	23	-0.0639	0.0639	0.0639	0.0000	Reach #9
16	9	23	-0.1188	0.1188	0.1188	0.0000	Reach #10
17	8	23	-0.1322	0.1322	0.1322	0.0000	Reach #11
18	7	23	-0.7256	0.7256	0.7256	0.0000	Reach #12
19	6	23	-0.7105	0.7105	0.7105	0.0000	Reach #13
20	5	23	-0.6214	0.6214	0.6214	0.0000	Reach #14
21	4	24	-0.3652	0.3652	0.3652	0.0000	Reach #15
22	3	24	-0.2737	0.2737	0.2737	0.0000	Reach #16
23	2	24	-0.1763	0.1763	0.1763	0.0000	Reach #17
24	5	6	-99.1196	99.1196	99.1196	0.0000	Obs Well #1
25	14	21	-99.0845	99.0845	99.0845	0.0000	Obs Well #2
26	22	18	-92.0838	92.0838	92.0838	0.0000	Obs Well #3
27	9	6	-5319.97	5,319.97	5,319.97	0.0000	Inj Well #1
28	14	24	-5312.39	5,312.39	5,312.39	0.0000	Inj Well #2
29	19	17	-5328.91	5,328.91	5,328.91	0.0000	Inj Well #3

Note : * Indicates the total concentration computed using the Eq. 3.8.1
: ** Indicates the simulated concentration using the aquifer transport simulation program developed.

The waste load demand specified within each time step is fully satisfied with the injection at the groundwater recharge wells, and at the surface water disposal locations, this is reflected in Table 5.1.16. Also, the minimum injection into the aquifer is satisfied. The injection concentration into the aquifer reached the upper bounds of the injection capacity only in the later time steps. The optimum concentration injection pattern was dictated by the maximum aquifer concentration allowed (of 100 mg/l) at the observation wells. These observation wells were placed in a radius of 750 m from the pumping wells as shown in Fig 5.1. The concentration at the pumping wells is well below the maximum specified. The maximum allowable concentration at the observation wells restricted the concentration reaching the pumping wells.

5.2 MANAGEMENT OF ONLY GROUNDWATER FLOW AND TRANSPORT WITH MULTIPLE REALIZATION OF HYDROGEOLOGIC PARAMETERS

The application discussed in the previous section (Section 5.1) consisted of using only a single realization of the hydrogeologic parameters, because of the limitation of the available computer memory. However, the model developed has no such limitations. As a demonstration to this another application of the management model developed is presented for the same aquifer described in Section 5.1 neglecting surface water flow and transport. All other data pertaining to boundary and initial conditions, locations of pumping wells, recharge wells, and observation wells are retained as previously. In this application five realizations of the hydrogeologic parameters are generated. The management model framed using multiple realizations minimizes the

uncertainty associated with the stochastically generated random fields. Maps of random stochastic fields of hydrogeologic parameters for realization 1, are the same as shown in Fig 5.3 through Fig 5.6. Samples of few other realizations generated are given in Appendix 6.

5.2.1 Groundwater Management for Water Quantity

The system and management constraint set for groundwater flow optimization are shown in Table 5.2.1. The control parameters describing the quantity optimization model for the 5 realizations used in here is given in Table 5.2.2.

Table 5.2.1

Constraints Used in Describing the Quantity Management Model

Description	Eq.No	Name	Type	Value
Limit on Aquifer Drawdowns	3.10.5	$s^*(k,NT)$	$\leq$	10.0 m
Minimum water demands to be satisfied	3.10.7	$D^*(i)$	$\geq$	5000 m^3/d
Cap on the pumping capacity	3.10.9	$Q_w^{max}(j,i$	$\leq$	3000 m^3/d

Table 5.2.2

Control Parameters for the Groundwater Management Model - Quantity

Description	Name	Value
Total number of decision variables	NDV	144
Total number of constraints	NTCE	1248
Number of non-linear equality constraints	NLEQ	0
Number of linear equality constraints	LEQ	0
Number of linear inequality constraints	LIEQ	1248

5.2.1.1 Discussion of Results for Groundwater Management

The management problem was solved using NEWSUMT-A non-linear optimization program. The optimized results for flow quantity is given in Table 5.2.3. The plot of aquifer piezometric heads obtained for realization #5 in the 24^{th} time step is shown in Fig 5.11. The optimum solution obtained here satisfied all the imposed management constraints, in all the realizations generated. The maximum permissible drawdown of 10.0 m is specified at each well locations. The drawdowns at each pumping well obtained using different realizations for the optimum solution in the 24^{th} time step are shown in Table 5.2.4. In the table, the drawdowns which are highlighted and underlined are the ones constraining any further improvement in the objective function.

Table 5.2.3

Optimized Results of Groundwater Pumping

WELL	LOCATION		WELL DISCHARGES IN CUBIC METERS PER DAY											
			TIME STEPS											
	ROW	COL	1	2	3	4	5	6	7	8	9	10	11	12
GW-1	3	6	1408	1408	1408	1408	1408	1408	1408	1408	1408	1408	1408	1408
GW-2	7	12	1013	1012	1012	1012	1012	1012	1012	1012	1012	1012	1012	1012
GW-3	9	17	833	833	833	833	833	833	833	833	833	833	833	833
GW-4	14	19	934	933	933	933	933	933	933	933	933	933	933	933
GW-5	19	24	1000	999	999	999	999	999	999	999	999	1000	1000	1000
GW-6	24	18	1019	1018	1018	1018	1018	1018	1018	1018	1018	1018	1018	1018
Total Well Discharges			6207	6203	6202	6202	6202	6202	6202	6202	6203	6203	6204	6205
Water Demand to be met			5000	5000	5000	5000	5000	5000	5000	5000	5000	5000	5000	5000

WELL	LOCATION		WELL DISCHARGES IN CUBIC METERS PER DAY											
			TIME STEPS											
	ROW	COL	13	14	15	16	17	18	19	20	21	22	23	24
GW-1	3	6	1408	1408	1408	1408	1408	1408	1408	1408	1408	1408	1408	1408
GW-2	7	12	1012	1013	1013	1013	1013	1013	1013	1013	1013	1013	1013	1013
GW-3	9	17	833	833	833	833	833	833	833	833	833	833	833	834
GW-4	14	19	933	934	934	934	934	934	934	934	934	934	934	934
GW-5	19	24	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1001	1001
GW-6	24	18	1019	1019	1019	1019	1019	1019	1019	1019	1019	1019	1019	1020
Total Well Discharges			6205	6206	6207	6207	6207	6207	6207	6207	6207	6207	6208	6209
Water Demand to be met			5000	5000	5000	5000	5000	5000	5000	5000	5000	5000	5000	5000

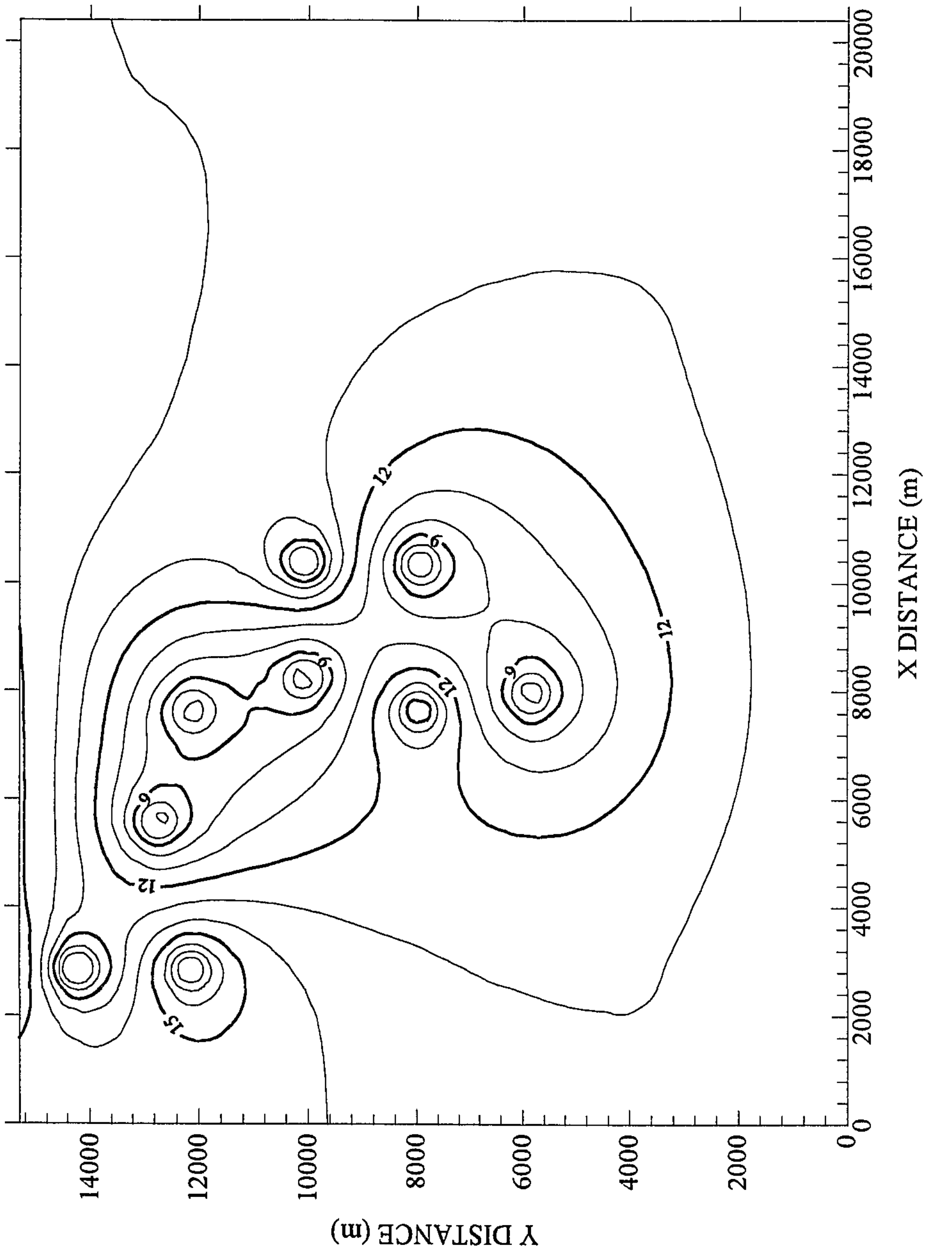


FIG 5.11: MAP OF AQUIFER HEADS (m) FOR REALIZATION #5

Table 5.2.4

Drawdowns at Groundwater Pumping Wells (24th time step)

Well No	Pumping Rate in 24 time step	Drawdowns in meters				
		RLZ-1	RLZ-2	RLZ-3	RLZ-4	RLZ-5
1	1408.1 m^3/d	**9.997**	9.081	9.108	8.856	8.524
2	1012.8 m^3/d	**9.996**	9.658	9.678	9.601	9.979
3	833.5 m^3/d	9.854	**9.996**	9.478	9.742	9.513
4	934.1 m^3/d	9.677	9.956	9.639	**9.995**	9.731
5	1007.7 m^3/d	9.699	9.756	9.821	9.712	**9.995**
6	1019.5 m^3/d	9.913	**9.996**	9.930	9.873	9.536

5.2.2 Groundwater Management of Water Quality

The unit-concentration response matrix is obtained by simulating for three potential injection wells over five realizations. The total number of simulation required were 360. The management constraints values pertaining to groundwater quality management is given in Table 5.2.5.

Table 5.2.5

Constraints Used in Describing Quality Management Model

Description	Eq. No	Name	Type	Value
Limit on groundwater pumping concentration	3.10.14	C_w^* (k,NT)	≤	2.0 mg/l
Limit on aquifer concentration at observation wells (750 m radius from the pumping well)	3.10.14	C_w^* (k,NT)	≤	100 mg/l
Minimum waste load demand to be satisfied	3.10.16	$WL^*(i)$	≥	Variable. Ranges from 3.0E6 to 1.0E7 g/d
Cap on the injection capacity	3.10.18	$C_w^{max}(j,i)$	≤	6000 mg/l

The control parameters describing optimization model for water quality are the number of decision variables equal to 72 and total number of constraints (all are linear inequality constraints) equal to 1176.

5.2.2.1 Discussion of Results for Groundwater Quality Management

The optimum concentration injection rates is given in Table 5.2.6. The plot of aquifer concentrations obtained for realization #5 in the 24th time step is shown in Fig 5.12. The optimum solution did satisfy all the imposed management constraints, in all the realizations used. As seen in Table 5.2.6 the concentration at injection wells reached its upper bound only in later time steps. The total waste load injected in 24 time periods in each recharge well was constrained by the maximum allowable concentration of 100 mg/l at observation wells. The concentrations at observation wells in the 24th time step for all the five realizations used is shown in Table 5.2.7.

Table 5.2.6

Optimized Results of Groundwater Concentration Injection Rates

Injection Well Location			CONCENTRATION INJECTION RATES (mg/l) TIME STEPS											
	ROW	COL	1	2	3	4	5	6	7	8	9	10	11	12
INJ-1	9	6	148	258	260	974	2883	5748	5983	5998	5997	5997	5997	5997
INJ-2	14	24	24	33	44	93	115	213	567	1488	3010	5842	5997	5996
INJ-3	19	17	2628	2822	3725	5098	5929	5997	5997	5996	5997	5998	5997	5997
Total Wasteload Injected			2.8E+06	3.1E+06	4.0E+06	6.2E+06	8.9E+06	1.2E+07	1.3E+07	1.3E+07	1.5E+07	1.8E+07	1.8E+07	1.8E+07
Min Injection Required			2.0E+06	3.0E+06	3.0E+06	3.0E+06	3.0E+06	3.0E+06	5.0E+06	5.0E+06	5.0E+06	5.0E+06	5.0E+06	5.0E+06

Injection Well Location			CONCENTRATION INJECTION RATES (mg/l) TIME STEPS											
	ROW	COL	13	14	15	16	17	18	19	20	21	22	23	24
INJ-1	9	6	5997	5997	5997	5997	5997	5997	5997	5997	5997	5997	5997	5997
INJ-2	14	24	5996	5997	5997	5997	5997	5997	5997	5997	5998	5997	5997	5998
INJ-3	19	17	5998	5997	5997	5998	5998	5998	5998	5997	5997	5998	5997	5997
Total Wasteload Injected			1.8E+07	1.8E+07	1.8E+07	1.8E+07	1.8E+07	1.8E+07	1.8E+07	1.8E+07	1.8E+07	1.8E+07	1.8E+07	1.8E+07
Min Injection Required			1.0E+07	1.0E+07	1.0E+07	1.0E+07	1.0E+07	1.0E+07	1.0E+07	1.0E+07	1.0E+07	1.0E+07	1.0E+07	1.0E+07

Note: Waste injection recharge rate at each injection well is specified as a constant and equal to 1000 m3/d.
Total Wasteload Injected and Min Injection Required are in grams/day.

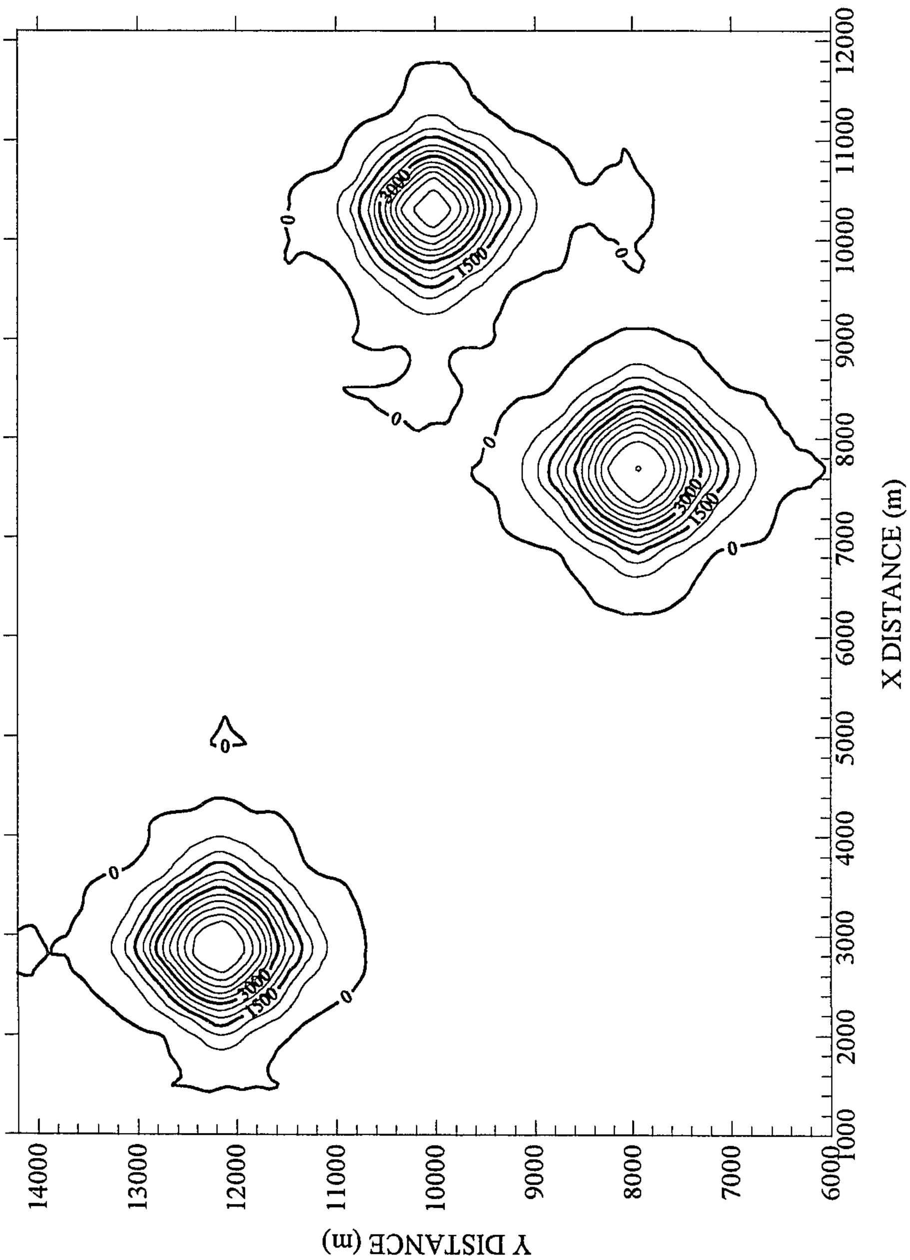


FIG 5.12: MAP OF AQUIFER CONCENTRATION (mg/l) FOR REALIZATION #5

In the table, the concentrations at observation wells which are highlighted and underlined are the ones constraining any further improvement in the objective function. As can be seen in the Table 5.2.7, Realization #1, #2, and #4 is not restricting or binding the optimum solution.

Table 5.2.7

Concentrations at Observation Wells (24th time step)

INJ Well No.	Total Waste Load Injected (Tons)	Concentration (mg/l) at Observation Wells				
		RLZ-1	RLZ-2	RLZ-3	RLZ-4	RLZ-5
1	35460	83.13	99.69	83.18	84.27	**99.99**
2	28620	74.70	87.28	**99.99**	85.38	96.23
3	40260	78.80	72.30	93.65	89.92	**99.99**

6. SUMMARY AND CONCLUSIONS

A mathematical model is developed based on a linked simulation-optimization procedure for comprehensive analysis and management of regional water resources. The control volume approach is utilized in the model development for the solution of groundwater flow and transport components, and surface water flow and transport components. The model exclusively incorporates hydraulic interaction of connected surface water groundwater systems. In the model streamflows and governing aquifer parameters are treated as stochastic random processes, and multiple realizations of the random field are generated and are incorporated in the management of the combined system.

The spatial variablility of hydrogeologic parameters, such as hydraulic conductivities in the X and Y directions and confined and unconfined storage coefficients are treated as stochastic random fields. It is assumed that the hydrogeologic parameters follow a log normal distribution, and the random field is characterized by a stationary exponential covariance function. The vector of the unknown spatial statistical structural parameters viz mean, variance, and the correlation length scales in the X and Y directions of the random field are determined by the maximum likelihood estimation (MLE) procedure. The Gaussian conditional mean estimates and conditional simulation are then employed to obtain multiple realizations of the random field. To generate the stochastic

random fields for real size problems, the model allows an option of dividing the entire domain into regions, whereby the computational efficiency is increased.

Implicit finite difference method is used in modeling the two-dimensional, horizontal flow equation under non-equilibrium conditions in a heterogeneous and anisotropic medium with known initial and boundary conditions. Iterative alternating direction implicit (IADI) method is used in its solution. The groundwater flow can be either confined or unconfined. Leaky aquifer conditions, groundwater evapotranspiration, and induced infiltration from surface water sources are incorporated into the aquifer flow simulation routine. The unit-response matrix approach (wherein the system responses for unit excitation at known potential well locations are recorded as unit-response functions) is used to accomplish the management goals. The simulation routine in generating unit-responses for imposed hydraulic stresses also accounts for boundary influences, and non-uniform initial conditions. The results of the flow simulation routine are in close agreement with analytical solutions, and numerical results of PLASM (Prickett and Lonnquist, 1971).

The piezometric heads obtained by flow simulation is used in defining groundwater velocities throughout the aquifer. These are then used in modeling the two-dimensional, unsteady groundwater solute transport process with known initial and boundary conditions. The solute transport process accounts for advection, diffusion, and dispersion of conservative and non-conservative substances with sources and/or sinks. The implicit centered finite difference is used in modeling the dispersive component. In accurately modeling the advective component four methods were tested viz (i) central, (ii) upwind, (iii) weighted difference, and (iv) quadratic upstream interpolation method. The

solution of the advection and dispersion components is obtained by IADI method. The unit-concentration response matrix approach (wherein the system responses for unit injection at known potential injection well locations are recorded as unit-concentration response functions) is used to accomplish the management goals. A unique approach is used in obtaining the unit-concentration response matrix for the non-equilibrium velocity field. The groundwater velocity field is well defined within each time step. This allows the governing pde (Eq. 3.6.1) to be linear within that time step. Therefore, in generating unit-concentration response matrix the process of generating response function by applying unit-injection in the first time step and recording the changes in concentration over the time period is repeated by applying unit-injection in each of the subsequent time steps and recording the changes in concentrations over the entire simulation period. The model solution of the solute transport process is verified and found to be in good agreement with known analytical solutions, and numerical results of method of characteristics (Konikow and Bredehoeft, 1978). Among the schemes tested for modeling advective component it was found quadratic upstream interpolation method as the best.

In modeling streams an option is available for specifying the inflow hydrograph to be either user defined or synthetically generated. The model generates a synthetic hydrograph based on the Markov process. Implicit finite difference method is used in modeling the one-dimensional surface water flow and transport processes. The surface water groundwater interaction, stream mass balance equations, and initial and boundary conditions are input to the management model as system constraints. The mass balance for each reach for each time step serves as a verification for surface water flow and transport processes.

A non-linear optimization program, NEWSUMT-A, developed by Thareja and Haftka (1985), is used in obtaining the solution of the management problem. For the case of aquifer management for flow and transport without streams the model gives an option to use either NEWSUMT-A or a linear programming optimization routine SIMPLEX. The optimum solution of NEWSUMT-A routine is verified by comparing it with optimum solution obtained by linear programming method (SIMPLEX). A dual programming management approach is utilized in optimizing flow quantities (well discharges and surface water diversions), and in determining optimal concentration injection pattern (injection rates through a set of recharge wells and surface water disposal rates). The constraint set for the management problem consists of system, environmental, and management constraints.

To demonstrate the application of the model, a hypothetical model is constructed based on a real physical system presented in the USGS Water-Resources Investigations Report (87-4240) on the Southeastern Virginia groundwater flow system. Most of the data used in the model application regarding hydrogeologic parameters, streamflow characteristics, boundaries of the aquifer, and location of major pumping centers pertains to Yorktown-Eastover aquifer, extracted from the above mentioned report. To demonstrate the various features built into the model two different scenarios are considered of the hypothetical model. In the first application a single realization of the hydrogeologic parameter field is generated for conjunctive-use management of groundwater flow and transport along with streamflows and solute transport in streams. The optimum solution obtained for this scenario did satisfy all the system and management constraints. The limitation on the available computer memory restricted the

application for a single realization of aquifer parameters. For this reason, a different scenario was considered for the same hypothetical model without the surface water component. In this second application five realizations of the hydrogeologic parameters were generated and the management was sought for flow and transport. The optimum solution obtained did satisfy all the system and management constraints imposed, in all the realizations generated.

6.1 FUTURE RESEARCH

The linked simulation-optimization procedure and the stochastic management model developed in this research work provides many useful tools for the efficient management and operation of a hydraulically connected surface water groundwater system. The modular approach is utilized in the development of the software program. This helps in expanding any module to incorporate additional features. One of the areas identified as a possible future research work is in parallel processing the generation of unit-response matrices. The generation of unit-response function for each potential pumping well or injection well is independent of other response functions being generated. Also, in the optimization routine as the number of decision variables and constraints increases, it would be advantageous to have parallel processing in generating derivatives of the constraints with respect to each decision variable by finite difference method, which is independent of all other operations. The same thing is true in generating the stochastic random fields, as each hydrogeologic parameter field is independent of the other, and for larger systems each region is independent of the other. This would certainly speed up the processing of larger systems with multiple realizations.

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A1. COMPUTATIONAL PROCEDURE FOR STOCHASTIC GENERATION OF AQUIFER PARAMETERS

In this appendix details of the maximum likelihood method and Gaussian conditional simulation are discussed. Reader is directed to Kitanidis and Lane (1985), and Wagner and Gorelick (1989) for a more detailed explanation on the procedure outlined here.

Defining the natural logarithm of a hydrogeologic parameter (hgp) at any point X_i as Y_i; the basic assumptions are

a. Y is normally distributed

b. Random log parameter Y is characterized by a stationary, exponential covariance function.

Then under these assumptions the mean and covariance for the random log field are:

$$E\,[Y_i] = \mu_Y \tag{A1.1}$$

$$Q = Cov\ (\xi) = \sigma_Y^2 \exp\left[-\left\{\left(\frac{\xi_1}{\lambda_1}\right)^2 + \left(\frac{\xi_2}{\lambda_2}\right)^2\right\}^{\frac{1}{2}}\right] \tag{A1.2}$$

where, E [ ] denotes expected value, Cov (ξ) = stationary anisotropic exponential covariance for two points separated by vector ξ , σ_Y^2 = variance of the random field, ξ_i = separation along dimensions i (i = 1,2), λ_i = correlation scale along dimension i.

The statistical structural parameters $\mu_y, \sigma_y^2, \lambda_x,\ and\ \lambda_y$ are denoted by a vector $\underline{\theta}$.

$$\underline{\theta} = \begin{bmatrix} \mu_y \\ \sigma_y^2 \\ \lambda_x \\ \lambda_y \end{bmatrix}$$

With this we can define the covariance matrix, Q, of the measured log parameters. Q is a symmetric matrix of size (NOM x NOM), where NOM is the number of measurements. Defining

$$T_{i,j} = \left[\left(\frac{\Delta x_{i,j}}{\lambda_x}\right)^2 + \left(\frac{\Delta y_{i,j}}{\lambda_y}\right)^2\right]^{\frac{1}{2}}$$

With the above definition, the (i,j) element of the covariance matrix Q can be expressed as

$$Q_{ij} = \sigma_y^2\ e^{-T_{ij}} \tag{A1.3}$$

It is intiutive to note the derivatives of the covariance matrix Q with respect to scalar structural parameters. We have

$$\frac{\partial Q}{\partial \mu} = 0 \tag{A1.4}$$

$$\left(\frac{\partial Q}{\partial \sigma^2}\right)_{i,j} = e^{-T_{ij}}, \quad i \neq j$$
$$= 1.0, \quad i = j \tag{A1.5}$$

$$\left(\frac{\partial Q}{\partial \lambda_x}\right)_{i,j} = \left(\frac{\Delta x_{ij}^2}{\lambda_x^3}\right)\left(\frac{1.0}{T_{ij}}\right) \sigma_y^2 \, e^{-T_{ij}}, \quad i \neq j$$
$$= 0.0, \quad i = j \tag{A1.6}$$

$$\left(\frac{\partial Q}{\partial \lambda_y}\right)_{i,j} = \left(\frac{\Delta y_{ij}^2}{\lambda_y^3}\right)\left(\frac{1.0}{T_{ij}}\right) \sigma_y^2 \, e^{-T_{ij}}, \quad i \neq j$$
$$= 0.0, \quad i = j \tag{A1.7}$$

The optimum structural parameters, $\underline{\theta}$, is obtained by the minimization of the negative log likelihood function

$$Min\ L(Z|\theta) = -\ln p(Z|\theta) = \frac{N}{2}\ln(2\pi) + \frac{1}{2}\ln|Q| + \frac{1}{2}(Z-\mu)^T Q^{-1}(Z-\mu) \tag{A1.8}$$

The optimum value of these unknown structural parameters lies at the extreme of the function, which is obtained by setting the derivative of negative log likelihood function with respect to each of the structural parameters to zero, i.e.,

$$\frac{\partial L}{\partial \mu} = 0; \quad \frac{\partial L}{\partial \sigma^2} = 0; \quad \frac{\partial L}{\partial \lambda_x} = 0; \quad \frac{\partial L}{\partial \lambda_y} = 0 \tag{A1.9}$$

The general expression for the derivative of the negative log likelihood function is

$$\frac{\partial L}{\partial \theta_j} = \frac{1}{2} Tr\left(Q^{-1} \frac{\partial Q}{\partial \theta_j} \right) - \frac{1}{2} (z-\mu)^T Q^{-1} \frac{\partial Q}{\partial \theta_j} Q^{-1} (z-\mu) - (z-\mu)^T Q^{-1} \frac{\partial \mu}{\partial \theta_j} \tag{A1.10}$$

where Tr = trace of a matrix in statistical terms, is a scalar quantity equal to sum of diagonal elements of a matrix. In writing the above expression, the following standard relations are used:

$$\frac{\partial \ln|Q|}{\partial \theta_j} = Tr\left[Q^{-1} \frac{\partial Q}{\partial \theta_j} \right] \tag{A1.11}$$

$$\frac{\partial Q^{-1}}{\partial \theta_j} = -Q^{-1} \frac{\partial Q}{\partial \theta_j} Q^{-1} \tag{A1.12}$$

Using the above general expression (Eq. A1.10), we can write

$$\frac{\partial L}{\partial \mu} = -(z-\mu)^T Q^{-1} \underline{1} \tag{A1.13}$$

$$\frac{\partial L}{\partial \sigma^2} = \frac{1}{2} Tr\left(Q^{-1} \frac{\partial Q}{\partial \sigma^2} \right) - \frac{1}{2} (z-\mu)^T Q^{-1} \frac{\partial Q}{\partial \sigma^2} Q^{-1} (z-\mu) \tag{A1.14}$$

$$\frac{\partial L}{\partial \lambda_x} = \frac{1}{2} Tr\left(Q^{-1} \frac{\partial Q}{\partial \lambda_x} \right) - \frac{1}{2} (z-\mu)^T Q^{-1} \frac{\partial Q}{\partial \lambda_x} Q^{-1} (z-\mu) \tag{A1.15}$$

$$\frac{\partial L}{\partial \lambda_y} = \frac{1}{2} Tr\left(Q^{-1} \frac{\partial Q}{\partial \lambda_y} \right) - \frac{1}{2} (z-\mu)^T Q^{-1} \frac{\partial Q}{\partial \lambda_y} Q^{-1} (z-\mu) \tag{A1.16}$$

The first-order necessary condition for the minimum $\underline{\theta}^*$, is that the

vector of derivatives is zero. That is for

$$g_j = \left(\frac{\partial L}{\partial \theta_j} \right)_{|\underline{\theta}=\underline{\theta}^*} \tag{A1.17}$$

$$\underline{g} = 0 \tag{A1.18}$$

A gradient based iterative method is used here to obtain the solution. The basic iteration is

$$\underline{\theta}_{i+1} = \underline{\theta}_i - \rho_i R_i g_i \tag{A1.19}$$

where $\underline{\theta}_i$ = vector of parameters in the i[th] iteration level; ρ_i = a scalar step-size parameter (here it is fixed, ρ_i = 1), and g_i is the gradient vector at i.

In the Gauss-Newton method employed here, R_i is the inverse of the Fisher Information Matrix (FIM). The elements of the FIM is defined as

$$M(j,k) = \frac{1}{2}\, Tr\left(Q^{-1} \frac{\partial Q}{\partial \theta_j} Q^{-1} \frac{\partial Q}{\partial \theta_k} \right) + \left(\frac{\partial \mu}{\partial \theta_j} \right)^T Q^{-1} \left(\frac{\partial \mu}{\partial \theta_k} \right) \tag{A1.20}$$

For four scalar parameters $\mu,\ \sigma^2,\ \lambda_x,\ and\ \lambda_y$, M is a (4 x 4) matrix. The sixteen elements of the matrix can be derived using the above general expression as:

$$M(\mu,\mu) = \underline{1}^T Q^{-1} \underline{1} \tag{A1.21}$$

$$M(\mu,\sigma^2) = 0 \tag{A1.22}$$

$$M(\mu, \lambda_x) = 0 \; ; \quad M(\mu, \lambda_y) = 0 \tag{A1.23}$$

$$M(\sigma^2, \mu) = 0 \tag{A1.24}$$

$$M(\sigma^2, \sigma^2) = \frac{1}{2} Tr\left(Q^{-1} \frac{\partial Q}{\partial \sigma^2} Q^{-1} \frac{\partial Q}{\partial \sigma^2} \right) \tag{A1.25}$$

$$M(\sigma^2, \lambda_x) = \frac{1}{2} Tr\left(Q^{-1} \frac{\partial Q}{\partial \sigma^2} Q^{-1} \frac{\partial Q}{\partial \lambda_x} \right) \tag{A1.26}$$

Likewise all the other elements are created, and the FIM is formed. The inverse of this matrix is, $R_i = M^{-1}$.

If the parameter estimates are highly correlated, the FIM is near singular and its inversion is impossible. In the computational procedure developed here, the FIM is first checked for singularity, in cases where it is near-singular the FIM is modified by first decomposing it into

$$M_i = S_i \; V_i \; S_i \tag{A1.27}$$

where subscript i refers to the iteration level, S_i is a diagonal matrix with the jj element equal to

$$(S_i)_{jj} = m_{jj}^{\frac{1}{2}} \tag{A1.28}$$

and V_i is the "correlation matrix", with the jk element equal to

$$(V_i)_{jk} = \frac{m_{jk}}{\sqrt{m_{jj}\ m_{kk}}} \tag{A1.29}$$

in which m denotes the elements of the FIM.

The eigenvalues (ev) of V_i are calculated. The condition number (CN), is then calculated as

$$CN = \frac{ev_{\max}}{ev_{\min}} \tag{A1.30}$$

If this condition number is greater than a user specified tolerance parameter (tpc), say 1000, then the CN is set equal to the tolerance parameter

$$\frac{ev_{\max}+Z}{ev_{\min}+Z} = tpc \tag{A1.31}$$

and Z is easily obtained. All the eigen values are increased by a positive constant Z and the correlation matrix V_i is modified accordingly. Using Eq. A1.30 a rescaled FIM is obtained.

Fig. A1.1 shows the flow chart used in the development of the Maximum Likelihood Estimation Procedure, and Fig. A1.2 shows the flow chart for generation of the multiple realizations using Gaussian conditional simulation.

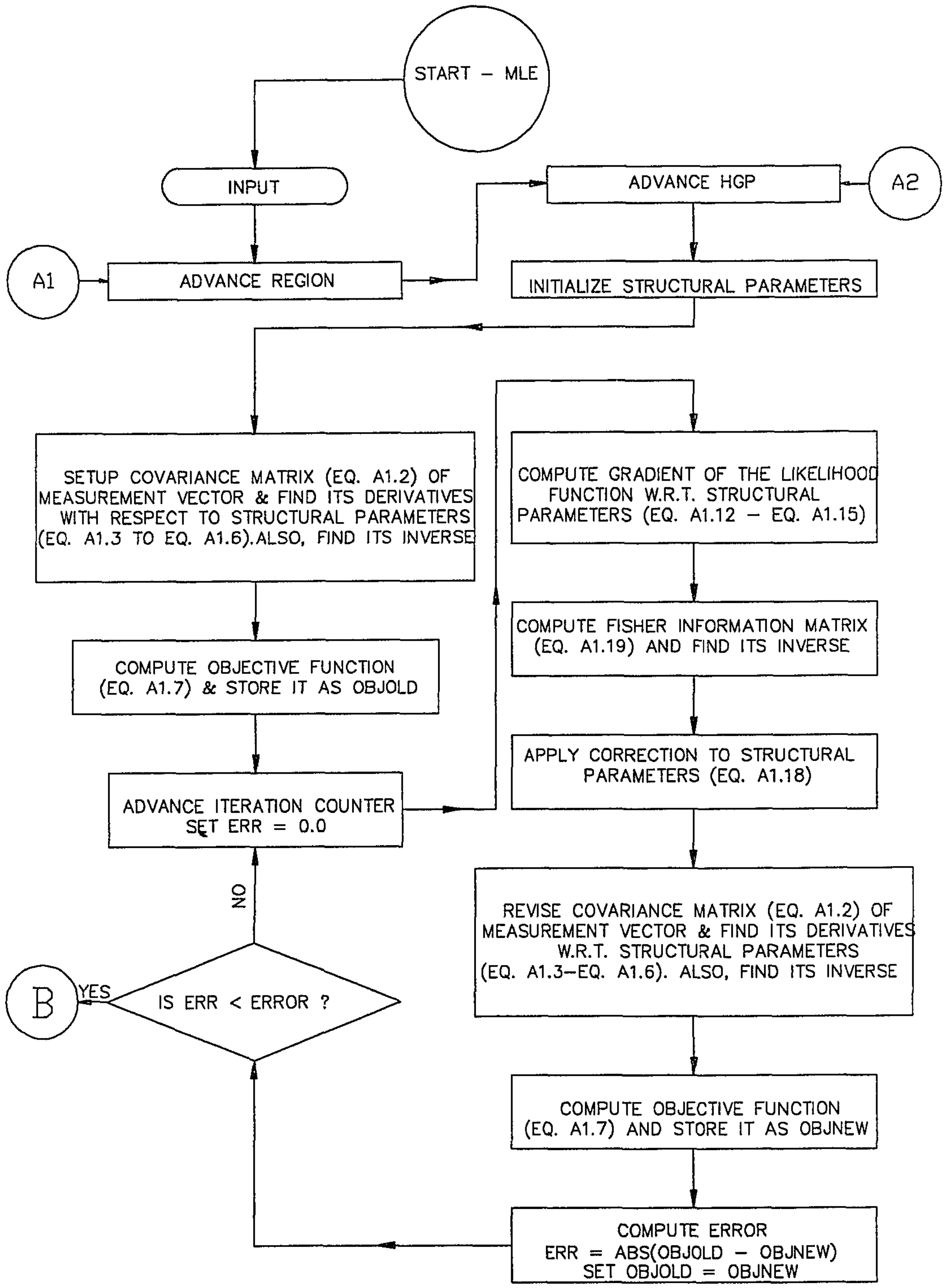


FIG A1.1: FLOW CHART FOR COMPUTATION OF MAXIMUM LIKELIHOOD ESTIMATION PROCEDURE

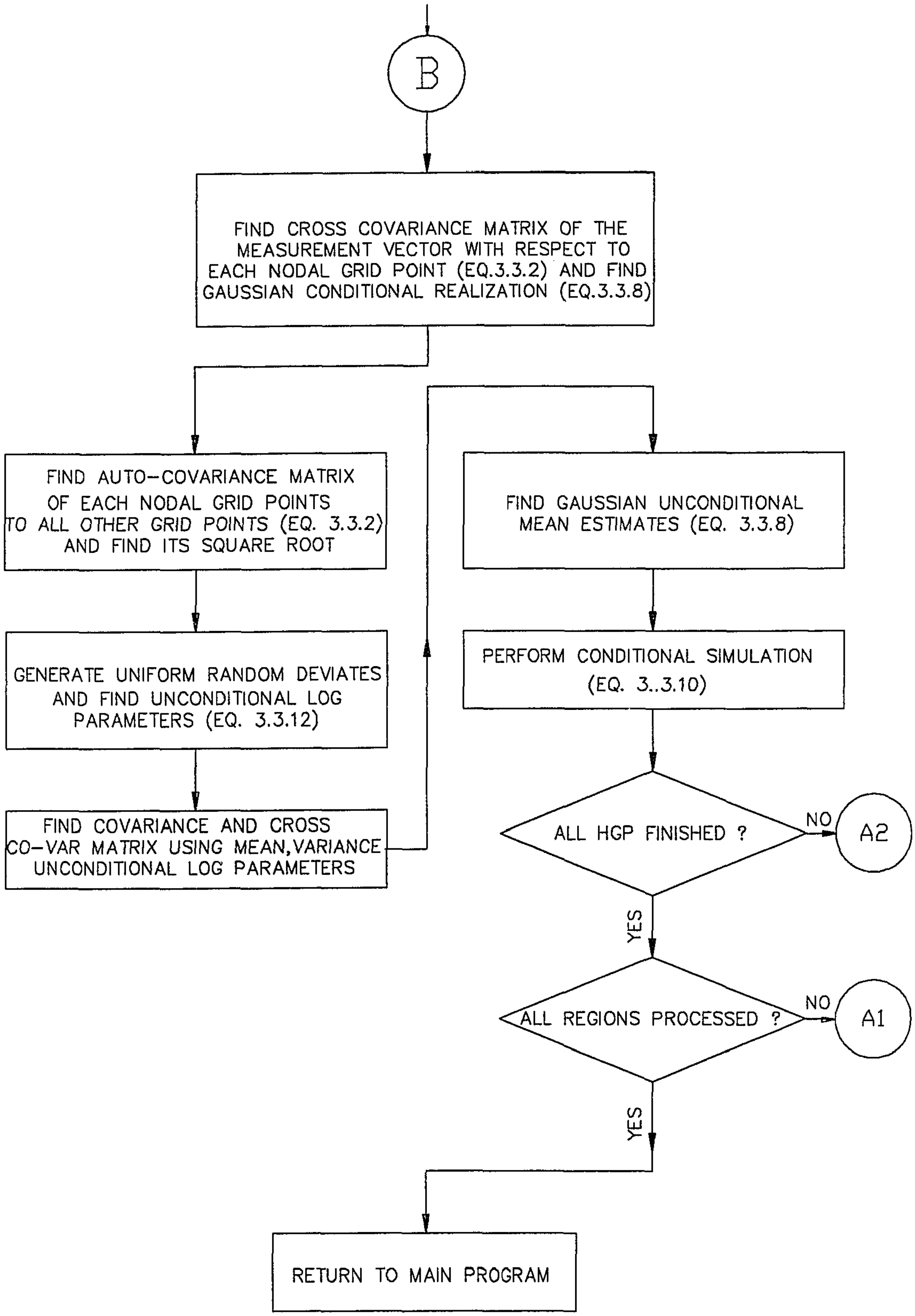


FIG A1.2: FLOW CHART FOR GAUSSIAN CONDITIONAL SIMULATION

A2. COMPUTATIONAL PROCEDURES FOR GROUNDWATER SOLUTE TRANSPORT USING UPSTREAM QUADRATIC INTERPOLATION FOR ADVECTIVE TERMS

In this appendix the development of upstream quadratic interpolation for a non-uniform grid is discussed. For a more detailed explanation of the steps involved, the reader is directed to B.P. Leonard (1979).

Refer to Fig. A2.1. In the figure $C_{f\,u/s}$, $C_{u/s}$, and $C_{d/s}$ stands for concentration at far upstream node, upstream node, and downstream node, respectively. For breivity hereafter referred to as C_f, C_u, and C_d. Also, Δ_f is the distance between the far upstream node and upstream node, and Δ_u is the distance between the upstream node and downstream node. Further, Z can either take X dimension or Y dimension.

Consider the general quadratic form

$$f = a\,Z^2 + b\,Z + c \tag{A2.1}$$

We have at $Z = 0$, $f = C_f$

at $Z = \Delta_f$, $f = C_u$

at $Z = (\Delta_f + \Delta_u)$, $f = C_d$

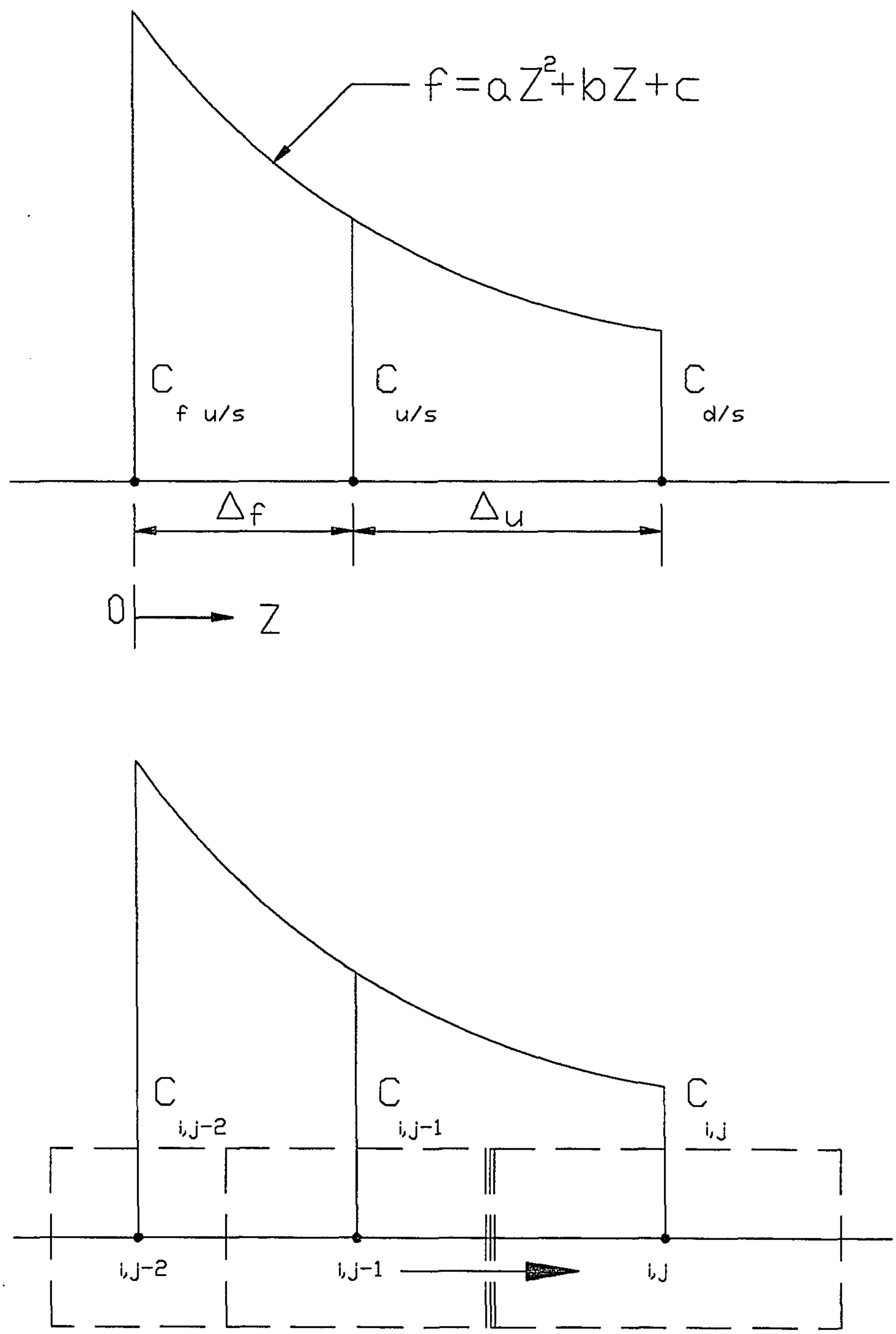


FIG A2.1: DEFINITION SKETCH FOR DETERMINING CELL WALL CONCENTRATION USING QUADRATIC UPSTREAM INTERPOLATION

Substituting these in the general expression given in Eq. A2.1, and solving for a, b, and c, we have

$$c = C_f$$

$$a = \frac{C_d\,\Delta_f - C_u\,\Delta_f - C_u\,\Delta_u + C_f\,\Delta_u}{\Delta_f\,(\Delta_u^2 + \Delta_f\,\Delta_u)} \tag{A2.2}$$

$$b = \frac{C_u - C_f - a\,\Delta_f^2}{\Delta_f}$$

Substituting for a, b, and c in the Eq. A2.1, we can write the most general expression of the quadratic function in one-dimension as

$$f = \left(\frac{C_d\,\Delta_f - C_u\,\Delta_f - C_u\,\Delta_u + C_f\,\Delta_u}{\Delta_f\,(\Delta_u^2 + \Delta_f\,\Delta_u)} \right) Z^2 + \left(\frac{C_u\,\Delta_u^2 + 2C_u\,\Delta_f\,\Delta_u - 2C_f\,\Delta_f\,\Delta_u - C_f\,\Delta_u^2 - C_d\,\Delta_f^2 + C_u\,\Delta_f^2}{\Delta_f\,(\Delta_u^2 + \Delta_f\,\Delta_u)} \right) Z + C_f \tag{A2.3}$$

To obtain the wall concentration of the Cell (i,j), concentrations of the two adjacent nodes to the wall under consideration together with one upstream node concentration will be used in the general quadratic expression Eq. A2.3.

For a uniform grid spacing $\Delta_f = \Delta_u = \Delta$, Eq. A2.3 reduces to

$$f = \left(\frac{C_d - 2C_u + C_f}{2\Delta^2} \right) Z^2 + \left(\frac{4C_u - 3C_f - C_d}{2\Delta} \right) Z + C_f \tag{A2.4}$$

To determine cell wall concentration, substitute Z as the distance from the far upstream node to the cell wall under consideration.

Grouping the terms in Eq. A2.3 we get

$$\left[\frac{\Delta_f Z^2 - \Delta_f^2 Z}{\Delta_f (\Delta_u^2 + \Delta_f\Delta_u)}\right] C_d + \left[\frac{-\Delta_f Z^2 - \Delta_u Z^2 + \Delta_u^2 Z + 2\Delta_f\Delta_u Z + \Delta_f^2 Z}{\Delta_f(\Delta_u^2 + \Delta_f\Delta_u)}\right] C_u + \left[\frac{\Delta_u Z^2 - 2\Delta_f\Delta_u Z - \Delta_u^2 Z + \Delta_f(\Delta_u^2+\Delta_f\Delta_u)}{\Delta_f(\Delta_u^2 + \Delta_f\Delta_u)}\right] C_f = f \tag{A2.5}$$

On the left hand side of Eq. A2.5, the terms in the brackets can be viewed as the weights associated with the concentrations $C_{d/s}$, $C_{u/s}$, and $C_{f\,u/s}$, respectively.

The weight, $W_{d/s}$, associated with downstream concentration is

$$W_{d/s} = \frac{\Delta_f Z^2 - \Delta_f^2 Z}{\Delta_f (\Delta_u^2 + \Delta_f\Delta_u)} \tag{A2.6}$$

The weight, $W_{u/s}$, associated with upstream concentration is

$$W_{u/s} = \frac{-\Delta_f Z^2 - \Delta_u Z^2 + \Delta_u^2 Z + 2\Delta_f\Delta_u Z + \Delta_f^2 Z}{\Delta_f(\Delta_u^2 + \Delta_f\Delta_u)} \tag{A2.7}$$

The weight, $W_{f\,u/s}$, associated with far upstream node concentration is

$$W_{f\,u/s} = \frac{\Delta_u Z^2 - 2\Delta_f\Delta_u Z - \Delta_u^2 Z + \Delta_f(\Delta_u^2+\Delta_f\Delta_u)}{\Delta_f(\Delta_u^2 + \Delta_f\Delta_u)} \tag{A2.8}$$

For the case of uniform grid spacing $\Delta_f = \Delta_u = \Delta$, and $Z = 1.5\ \Delta$, evaluating the funtion, f, at the cell wall under consideration, Eq. A2.5 reduces to

$$f = 0.375\, C_{d/s} + 0.75\, C_{u/s} - 0.125\, C_{f\,u/s} \tag{A2.9}$$

Eq. A2.9 is formally equivalent to

$$C_{i,j\pm\frac{1}{2}} \text{ or } C_{i\pm\frac{1}{2},j} = \frac{1}{2}(C_u + C_d) - \frac{1}{8}(C_f - 2C_u + C_d) \tag{A2.10}$$

On the right hand side of Eq. A2.10, the first term corresponds to the linear interpolation of upstream and downstream concentrations, and the second term corresponds to the correction applied to account for curvature effects.

Depending on the flow direction, one can construct two distinct cases for each face of the cell. In all there would be eight cases. The two cases for each of the left and right faces are shown in Fig. A2.2, and the two cases for each of the top and bottom faces are shown in Fig. A2.3. Description of the eight cases are given below:

<u>Case 1:</u> Left Face

Flow Direction: Left to Right

In the general expression (Eq. A2.5) substitute,

$C_f = C_{i,j-2}$, $C_u = C_{i,j-1}$, and $C_d = C_{i,j}$

$$\Delta_f = \frac{\Delta x_{j-2} + \Delta x_{j-1}}{2}, \quad \Delta_u = \frac{\Delta x_{j-1} + \Delta x_j}{2}, \quad Z = \frac{\Delta x_{j-2}}{2} + \Delta x_{j-1}$$

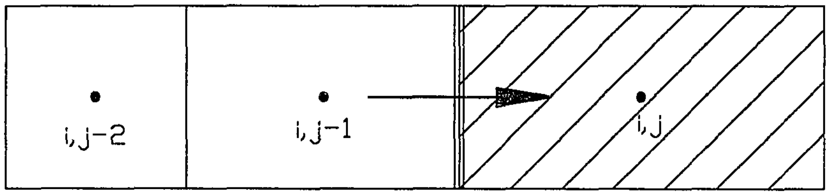
<u>Case 2:</u> Left Face

Flow Direction: Right to Left

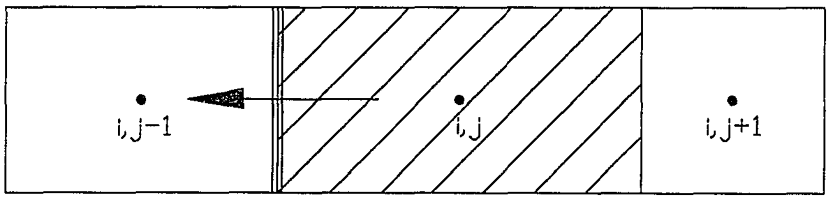
In the general expression (Eq. A2.5) substitute,

$C_f = C_{i,j+1}$, $C_u = C_{i,j}$, and $C_d = C_{i,j-1}$

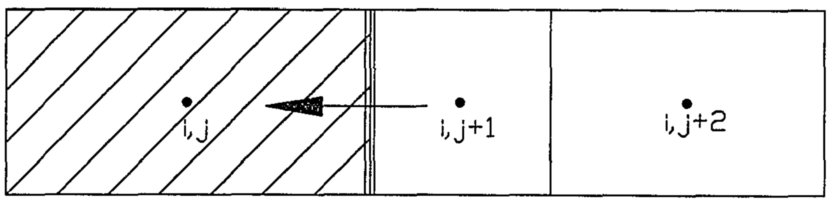
$$\Delta_f = \frac{\Delta x_{j+1} + \Delta x_j}{2}, \quad \Delta_u = \frac{\Delta x_{j-1} + \Delta x_j}{2}, \quad Z = \frac{\Delta x_{j+1}}{2} + \Delta x_j$$



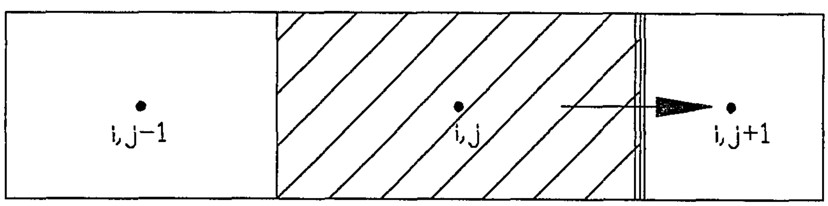
Case 1: Left face, flow left to right



Case 2: Left face, flow right to left

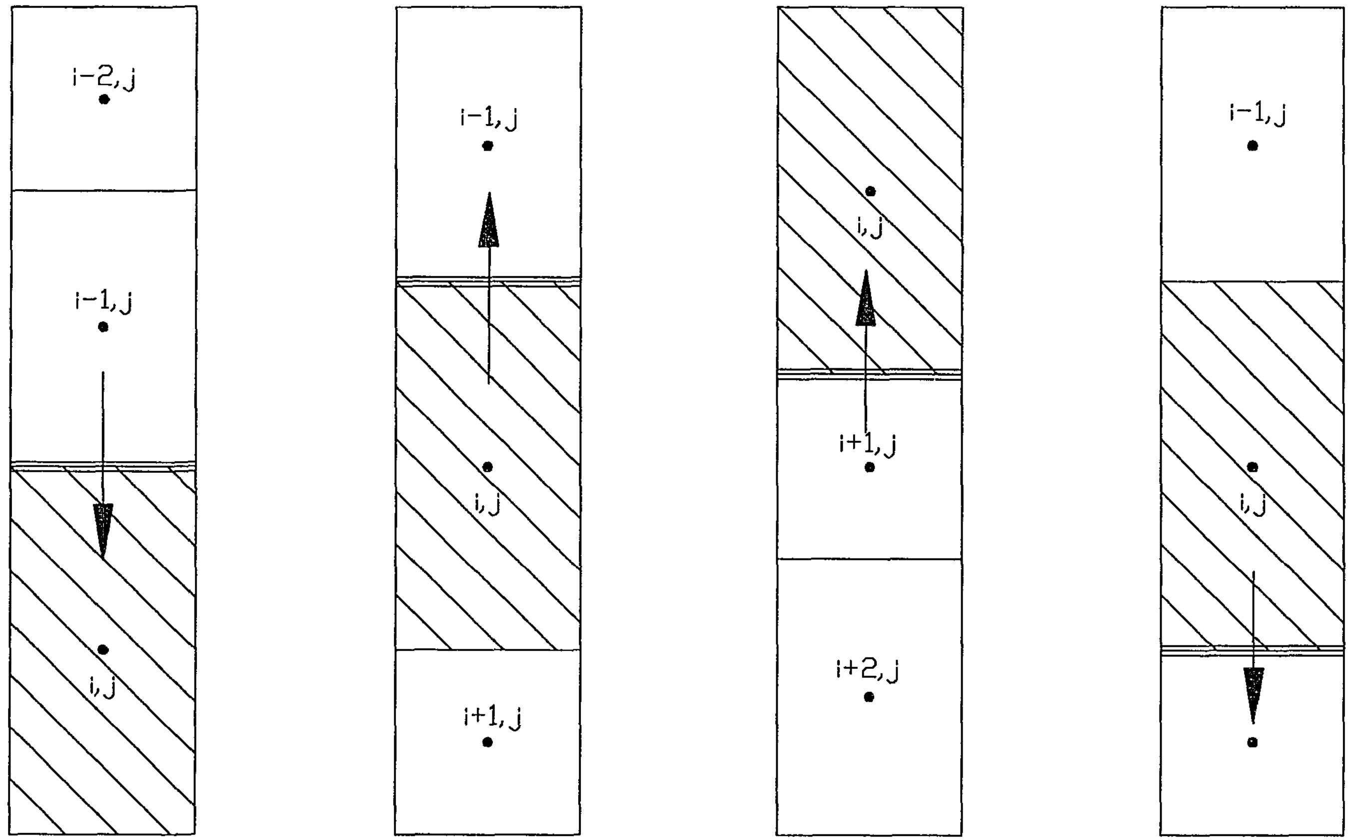


Case 3: Right face, flow right to left



Case 4: Right face, flow left to right

FIG. A2.2: SCHEMATIC OF QUADRATIC UPSTREAM INTERPOLATION FOR ADVECTIVE TERMS IN X-DIRECTION



Case 5
Top face
flow top to bottom

Case 6
Top face
flow bottom to top

Case 7
Bottom face
flow bottom to top

Case 8
Bottom face
flow top to bottom

FIG. A2.3: SCHEMATIC OF QUADRATIC UPSTREAM INTERPOLATION
FOR ADVECTIVE TERMS IN Y-DIRECTION

Case 3: Right Face

Flow Direction: Right to Left

In the general expression (Eq. A2.5) substitute,

$C_f = C_{i,j+2}$, $C_u = C_{i,j+1}$, and $C_d = C_{i,j}$

$$\Delta_f = \frac{\Delta x_{j+1} + \Delta x_{j+2}}{2}, \quad \Delta_u = \frac{\Delta x_{j+1} + \Delta x_j}{2}, \quad Z = \frac{\Delta x_{j+2}}{2} + \Delta x_{j+1}$$

Case 4: Right Face

Flow Direction: Left to Right

In the general expression (Eq. A2.5) substitute,

$C_f = C_{i,j-1}$, $C_u = C_{i,j}$, and $C_d = C_{i,j+1}$

$$\Delta_f = \frac{\Delta x_{j-1} + \Delta x_j}{2}, \quad \Delta_u = \frac{\Delta x_j + \Delta x_{j+1}}{2}, \quad Z = \frac{\Delta x_{j-1}}{2} + \Delta x_j$$

Case 5: Top Face

Flow Direction: Top to Bottom

In the general expression (Eq. A2.5) substitute,

$C_f = C_{i-2,j}$, $C_u = C_{i-1,j}$, and $C_d = C_{i,j}$

$$\Delta_f = \frac{\Delta y_{i-2} + \Delta y_{i-1}}{2}, \quad \Delta_u = \frac{\Delta y_{i-1} + \Delta y_i}{2}, \quad Z = \frac{\Delta y_{i-2}}{2} + \Delta y_{i-1}$$

Case 6: Top Face

Flow Direction: Bottom to Top

In the general expression (Eq. A2.5) substitute,

$C_f = C_{i+1,j}$, $C_u = C_{i,j}$, and $C_d = C_{i-1,j}$

$$\Delta_f = \frac{\Delta y_{i+1} + \Delta y_i}{2}, \quad \Delta_u = \frac{\Delta y_{i-1} + \Delta y_i}{2}, \quad Z = \frac{\Delta y_{i+1}}{2} + \Delta y_i$$

Case 7: Bottom Face

Flow Direction: Bottom to Top

In the general expression (Eq. A2.5) substitute,

$C_f = C_{i+2,j}$, $C_u = C_{i+1,j}$, and $C_d = C_{i,j}$

$$\Delta_f = \frac{\Delta y_{i+2} + \Delta y_{i+1}}{2}, \quad \Delta_u = \frac{\Delta y_{i+1} + \Delta y_i}{2}, \quad Z = \frac{\Delta y_{i+2}}{2} + \Delta y_{i+1}$$

Case 8: Bottom Face

Flow Direction: Top to Bottom

In the general expression (Eq. A2.5) substitute,

$C_f = C_{i-1,j}$, $C_u = C_{i,j}$, and $C_d = C_{i+1,j}$

$$\Delta_f = \frac{\Delta y_{i-1} + \Delta y_i}{2}, \quad \Delta_u = \frac{\Delta y_{i+1} + \Delta y_i}{2}, \quad Z = \frac{\Delta y_{i-1}}{2} + \Delta y_i$$

The dispersion component of the transport process is the same as explained in Section 3.6.2. For clarity the finite difference equations for dispersion component is repeated here.

Dispersive fluxes entering a finite difference cell from all the four sides is considered in writing expression for mass conserving over the element.

Dispersive input in X direction entering the Cell (i,j) from left face

$= Dxx1\ (C_{i,j-1} - C_{i,j})$ (A2.11)

Dispersive input in X direction entering the Cell (i,j) from right face

$= Dxx3\ (C_{i,j+1} - C_{i,j})$ (A2.12)

Dispersive input in Y direction entering the Cell (i,j) from top face

$= Dyy2\ (C_{i-1,j} - C_{i,j})$ (A2.13)

Dispersive input in Y direction entering the Cell (i,j) from bottom face

$= Dyy4\ (C_{i+1,j} - C_{i,j})$ (A2.14)

In the computation of groundwater solute transport component, the piezometric heads obtained from the flow simulation is used to define velocities $Uxx_{i,j}$ and $Uyy_{i,j}$ throughout the grid for each time step (ref Fig. 3.6). The velocities $Uxx_{i,j}$ and $Uyy_{i,j}$ are defined at the right face and top face of each finite difference cell, and are expressed by:

$$Uxx_{i,j} = \left(\frac{Kx_{i,j} + Kx_{i,j+1}}{2} \right) \frac{h_{i,j} - h_{i,j+1}}{\left(\frac{\Delta x_j + \Delta x_{j+1}}{2} \right)} \qquad \text{(A2.15)}$$

Similarly,

$$Uyy_{i,j} = \left(\frac{Ky_{i,j} + Ky_{i-1,j}}{2} \right) \frac{h_{i,j} - h_{i-1,j}}{\left(\frac{\Delta y_i + \Delta y_{i-1}}{2} \right)} \qquad \text{(A2.16)}$$

The mass of solute transported by way of advection is a product of flow and concentration entering the Cell (i,j) through each of the four faces. The flow term in the advective component can be written as

Flow entering the aquifer from the left face

$$T1 = + Uxx_{i,j-1}\ \Delta y_i \left(\frac{b_o + b_1}{2} \right) \tag{A2.17}$$

Flow entering the aquifer from the right face

$$T3 = - Uxx_{i,j}\ \Delta y_i \left(\frac{b_o + b_3}{2} \right) \tag{A2.18}$$

Flow entering the aquifer from the top face

$$T2 = - Uyy_{i,j}\ \Delta x_j \left(\frac{b_o + b_2}{2} \right) \tag{A2.19}$$

Flow entering the aquifer from the bottom face

$$T4 = + Uyy_{i+1,j}\ \Delta x_j \left(\frac{b_o + b_4}{2} \right) \tag{A2.20}$$

Advective component in X direction, for mass entering the Cell (i,j) from left face

$$AD1 = T1(W_{10}C_{i,j}+W_{11}C_{i,j-1}+W_{12}C_{i,j-2}+W_{13}C_{i,j+1}+W_{14}C_{i,j+2}) \tag{A2.21}$$

Advective component in X direction, for mass entering the Cell (i,j) from right face

$$AD3 = T3(W_{30}C_{i,j}+W_{31}C_{i,j-1}+W_{32}C_{i,j-2}+W_{33}C_{i,j+1}+W_{34}C_{i,j+2}) \tag{A2.22}$$

Advective component in Y direction, for mass entering the Cell (i,j) from top face

$$AD2 = T2(W_{20}C_{i,j}+W_{21}C_{i-1,j}+W_{22}C_{i-2,j}+W_{23}C_{i+1,j}+W_{24}C_{i+2,j}) \tag{A2.23}$$

Advective component in Y direction, for mass entering the Cell (i,j) from bottom face

$$AD4 = T4(W_{40}C_{i,j}+W_{41}C_{i-1,j}+W_{42}C_{i-2,j}+W_{43}C_{i+1,j}+W_{44}C_{i+2,j}) \tag{A2.24}$$

Depending on the flow direction at the cell wall, only three weights associated with downstream, upstream, and far upstream are defined in the Eq. A2.21 through A2.24 (the weights are defined in Eq. A2.6 through A2.8). The remaining two weights are assigned a value zero as the case may be.

As in the case of groundwater flow component, the block centered finite difference formulation for dispersive component and quadratic upstream interpolation formulation for advective component for the governing advection-dispersion equation given in Eq. 3.6.1, follows from the application of continuity of mass: sum of all mass flow rates into and out of a Cell (i,j) that has sides Δx_j and Δy_i must equal rate of change of mass in the aquifer element.

$$\begin{aligned}
&Dxx1\ (C^{n+1}_{i,j-1} - C^{n+1}_{i,j}) + Dxx3\ (C^{n+1}_{i,j+1} - C^{n+1}_{i,j}) + \\
&Dyy2\ (C^{n+1}_{i-1,j} - C^{n+1}_{i,j}) + Dyy4\ (C^{n+1}_{i+1,j} - C^{n+1}_{i,j}) + \\
&T1\ (W_{10}C^{n+1}_{i,j} + W_{11}C^{n+1}_{i,j-1} + W_{12}C^{n+1}_{i,j-2} + W_{13}C^{n+1}_{i,j+1} + W_{14}C^{n+1}_{i,j+2}) + \\
&T3\ (W_{30}C^{n+1}_{i,j} + W_{31}C^{n+1}_{i,j-1} + W_{12}C^{n+1}_{i,j-2} + W_{13}C^{n+1}_{i,j+1} + W_{14}C^{n+1}_{i,j+2}) + \\
&T2\ (W_{20}C^{n+1}_{i,j} + W_{21}C^{n+1}_{i-1,j} + W_{22}C^{n+1}_{i-2,j} + W_{23}C^{n+1}_{i+1,j} + W_{24}C^{n+1}_{i+2,j}) + \\
&T4\ (W_{40}C^{n+1}_{i,j} + W_{41}C^{n+1}_{i-1,j} + W_{42}C^{n+1}_{i-2,j} + W_{43}C^{n+1}_{i+1,j} + W_{44}C^{n+1}_{i+2,j}) - \\
&d_k(\phi\ b_{i,j}\Delta x_j\ \Delta y_i)\, C^{n+1}_{i,j} + C'_{i,j}Q'_{i,j} - Qw_{i,j}C^{n+1}_{i,j} \\
&\qquad = (\phi\ b_{i,j}\Delta x_j\ \Delta y_i)\left(\frac{C^{n+1}_{i,j} - C^{n}_{i,j}}{\Delta t} \right)
\end{aligned} \tag{A2.25}$$

where ϕ is the aquifer porosity, W's are the weights associated as the case may be on

the downstream, upstream and far upstream, d_k is the decay rate [1/T], Q_w is the groundwater pumping associated with the node (i,j), C' and Q' are the concentration and waste discharge rate of the external sources, n is the time step.

APPENDIX A3

FLOW CHART FOR AQUIFER FLOW AND TRANSPORT SIMULATION

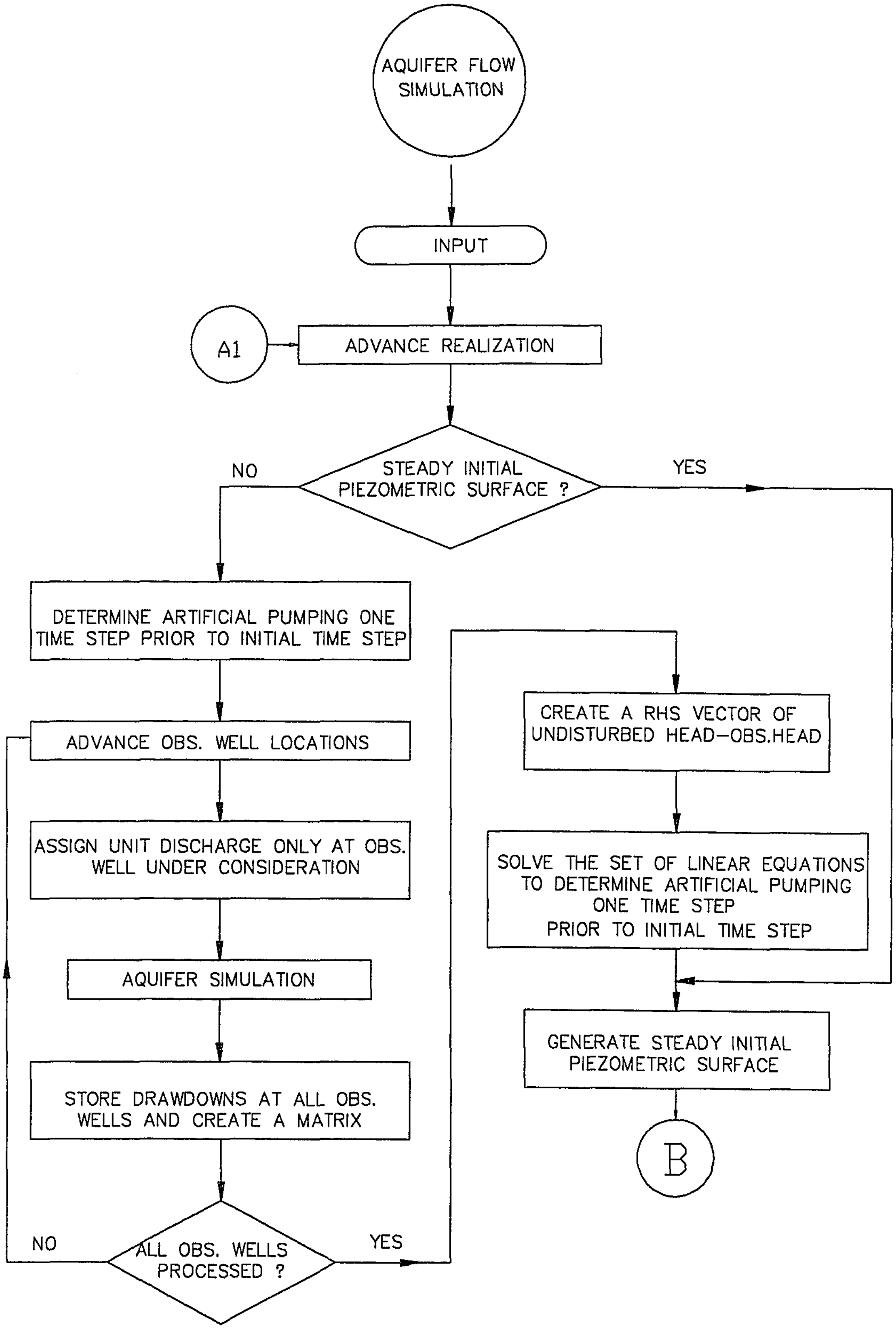


FIG A3.1: FLOW CHART FOR GROUNDWATER FLOW SIMULATION MODEL

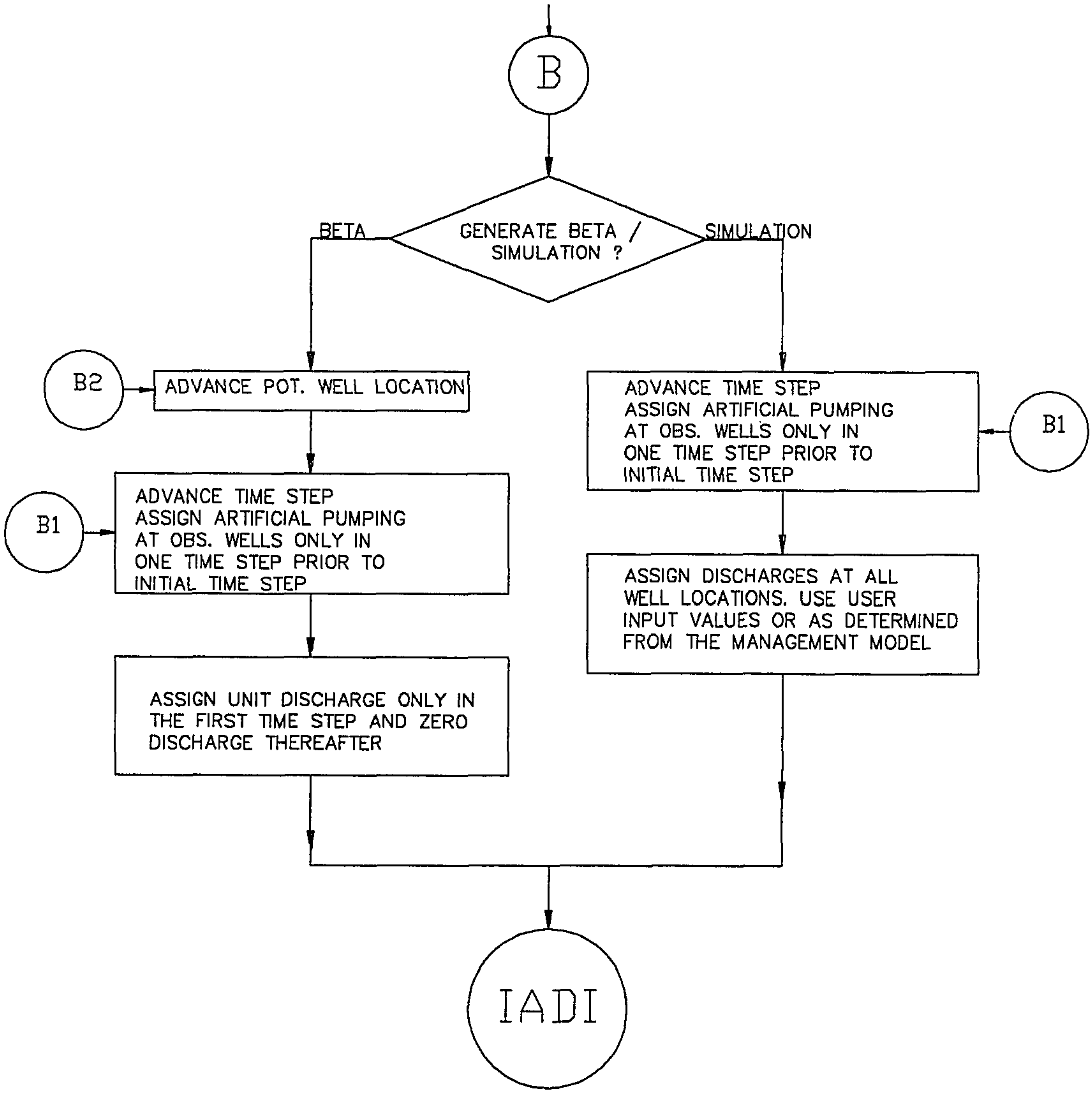


FIG A3.1: FLOW CHART FOR GROUNDWATER FLOW SIMULATION MODEL
(CONTINUED)

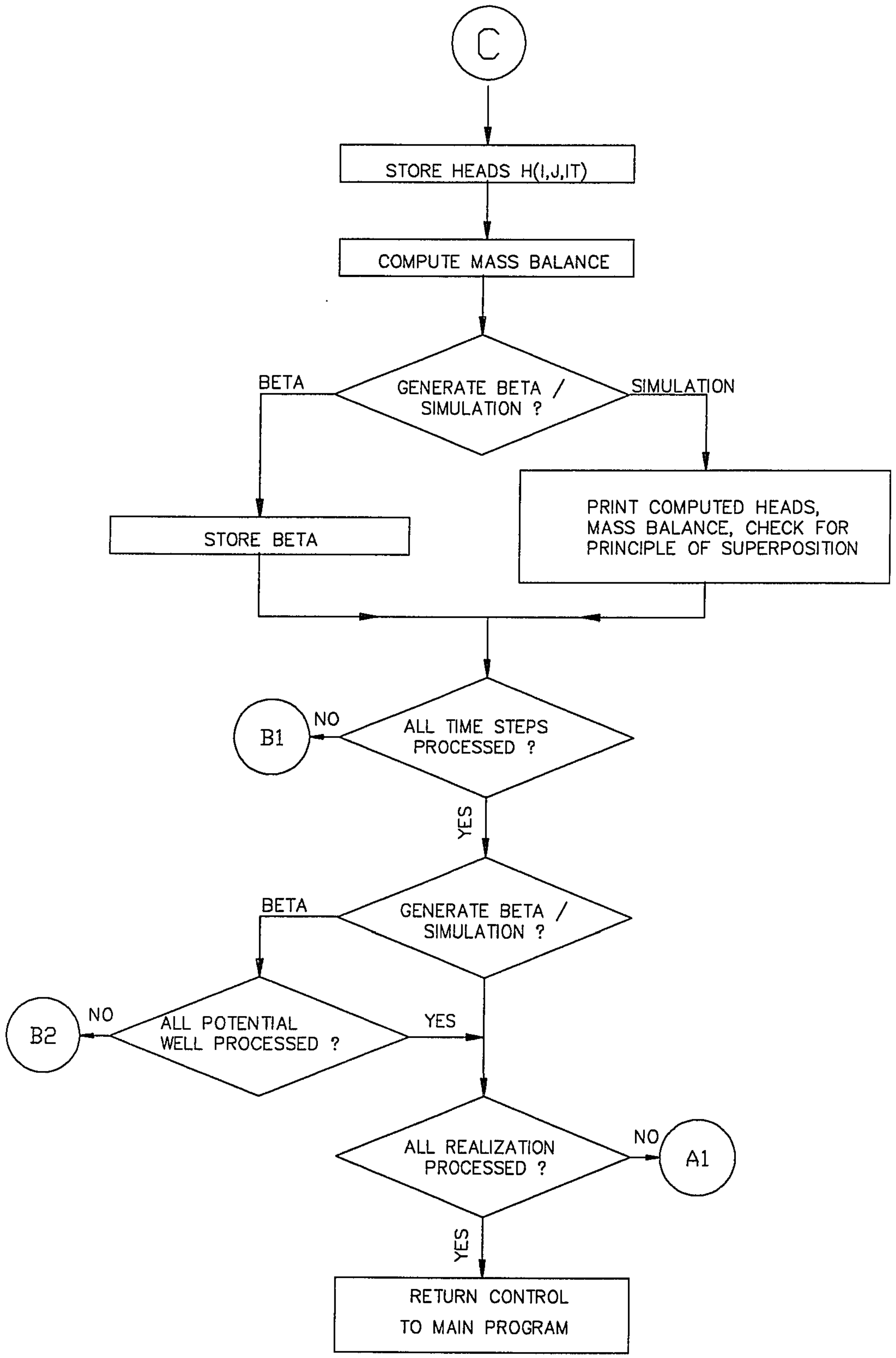


FIG A3.1: FLOW CHART FOR GROUNDWATER FLOW SIMULATION MODEL (CONTINUED)

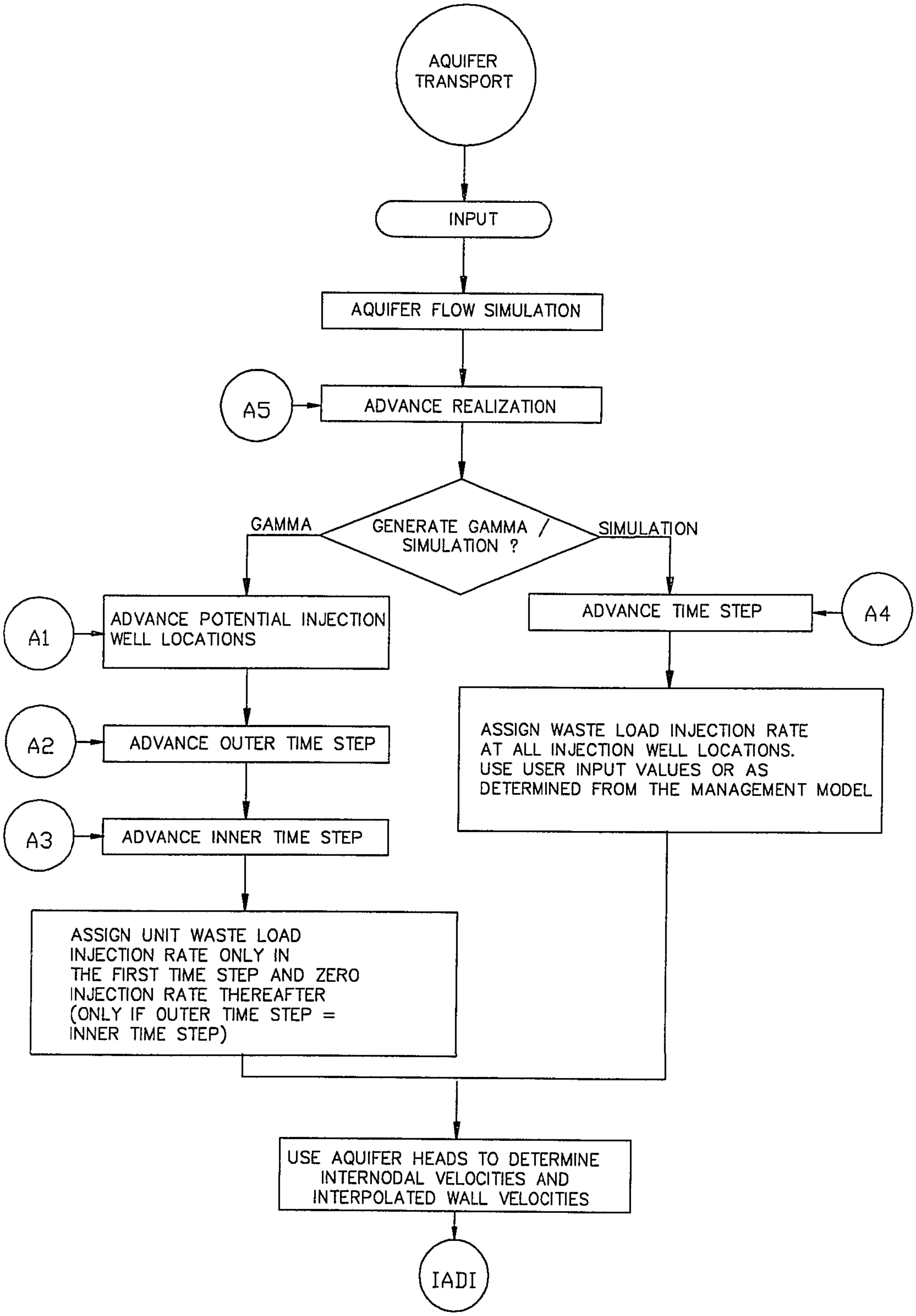


FIG A3.2: FLOW CHART FOR SOLUTE TRANSPORT SIMULATION MODEL

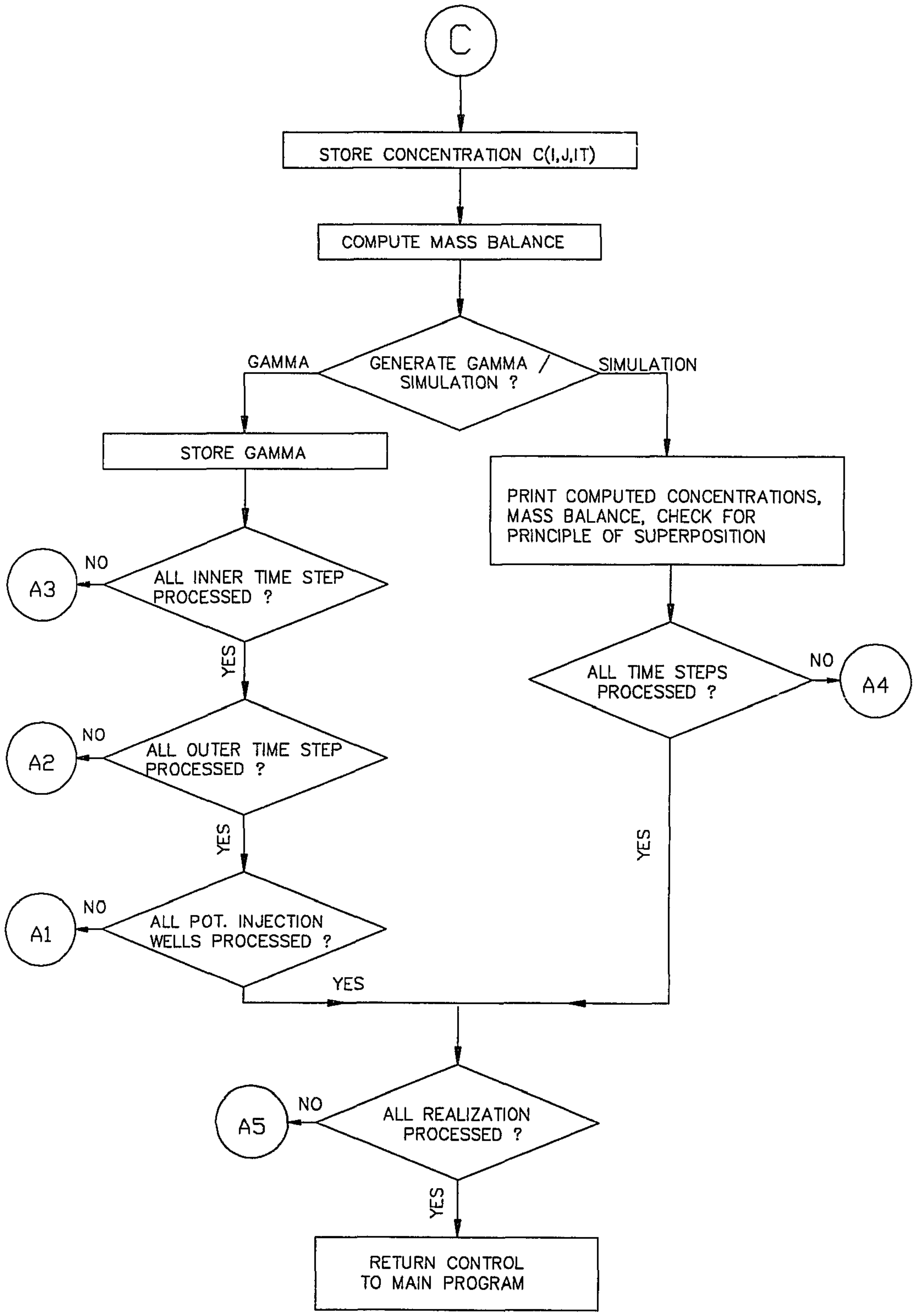


FIG A3.2: FLOW CHART FOR SOLUTE TRANSPORT SIMULATION MODEL (CONTINUED)

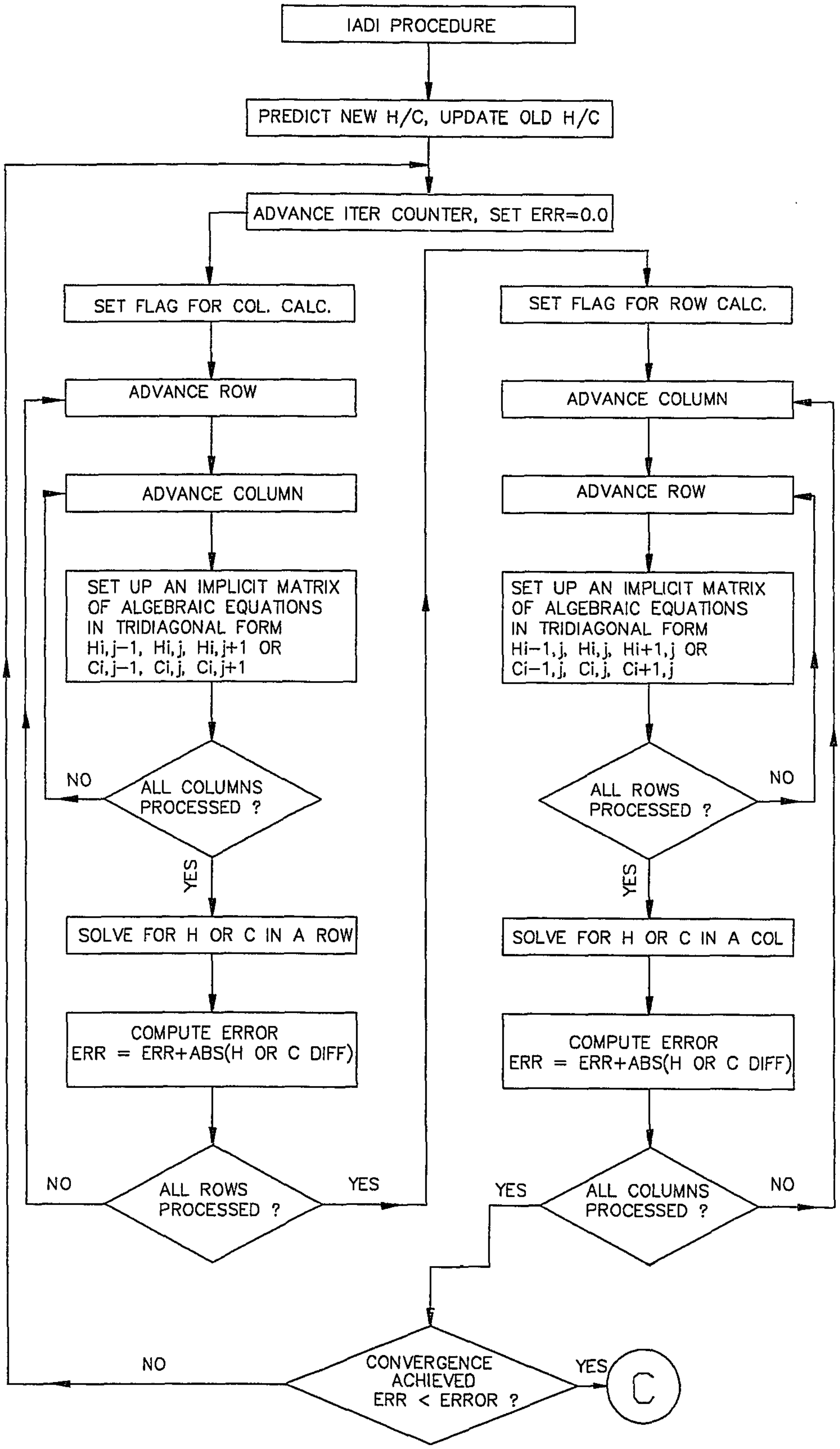


FIG A3.3: FLOW CHART FOR IADI PROCEDURE

A4. COMPUTATIONAL PROCEDURE OF NEWSUMT - A

The optimization program used in this research work is NEWSUMT-A developed by Rajiv Thareja and Raphael T. Haftka (1985). In this appendix computational procedure of NEWSUMT-A adopted in their work is briefly discussed. For a more detailed explanation of the algorithm, steps and features incorporated in their model, the reader is directed to the software user manual for NEWSUMT-A.

NEWSUMT-A is a non-linear optimization computer program written in standard FORTRAN subroutine form for the solution of linear and non-linear equality and/or inequality constrained or unconstrained function minimization problems. The minimization algorithm used in NEWSUMT-A is a sequence of unconstrained minimizations technique (SUMT).

Optimization problems must be formulated in the following canonical form when NEWSUMT-A program is used:

Minimize the objective function

$$\text{Min } Z = f(x_1,x_2,x_3,\ldots\ldots x_n) \qquad \text{(A4.1)}$$

Subject to a set of inequality and/or equality constraints

$$g_q(x_1,x_2,x_3,\ldots\ldots x_n) \;\geq\; 0, \text{ and/or} \qquad \text{(A4.2)}$$

$$h_q(x_1,x_2,x_3,\ldots\ldots x_n) = 0 \qquad \text{(A4.3)}$$

and the side bound on the design variables

$$x_j^L \leq x_j \leq x_j^U \tag{A4.4}$$

where the functions f(X), g_q(X), and h_q(X) are continuous and differentiable real functions with respect to the design variables x_j, j = 1,2,3,...,NDV.

In using NEWSUMT-A program, user has to model Eq. A4.1 through Eq. A4.4, and, if available, the derivatives of Eq. A4.1 through Eq. A4.3 (if derivatives are not available NEWSUMT-A determines it using standard finite difference approximations) in a subroutine form. NEWSUMT-A program calls the user defined subroutine to evaluate the functions iteratively. Also, initial design variables needs to be specified. NEWSUMT-A then systematically modifies these while generating a sequence of vectors X^i so that f(X) decreases or the degree of constraint satisfaction is improved. This sequence of vectors X converge to a solution X^* where the constraint violation is very small and f(X^*) is at least a local minimum.

APPENDIX A5

INPUT DATA FILE FOR CONJUNCTIVE-USE MANAGEMENT MODEL APPLICATION

```
Yorktown-Eastover Aquifer Characteristics - Stochastic Generation
17 River Reaches for James River - MANAGEMENT FOR QUANTITY, & QUALITY
Six Pumping Wells & three injection Wells, Fine Tuning, Variable
Velocity Field
Revised Run #5, Created on 04/16/96  24 TIME STEPS, Time Period 300 days
0  0  0  1  1  1  0  1  0  0  1
34  41  1
600.  600.  600.  600.  300.  300.  300.  600.  600.  600.
300.  300.  300.  600.  600.  300.  300.  300.  300.  300.
600.  600.  300.  300.  300.  600.  600.  600.  600.  600.
600.  600.  600.  600.  600.  600.  600.  600.  600.  600.
600.
600.  300.  300.  300.  600.  300.  300.  300.  300.  300.
600.  600.  300.  300.  300.  600.  600.  300.  300.  300.
600.  600.  300.  300.  300.  600.  600.  600.  600.  600.
600.  600.  600.  600.
4  4  4
  9  1  1 17 20
 12  1 21 17 41
  8 18  1 34 20
 11 18 21 34 41
   4   3   4.3   4.3   6.4E-06   1.1E-01
   4   9   5.1   4.9   8.0E-06   1.3E-01
   4  15   5.3   5.3   7.0E-06   1.9E-01
   9   3   4.1   4.1   7.2E-06   1.6E-01
   9   9   4.5   4.5   8.0E-06   1.0E-01
   9  15   4.5   4.5   6.5E-06   1.3E-01
  14   3   4.1   4.1   7.2E-06   2.5E-01
  14   9   4.4   4.4   7.3E-06   1.8E-01
  14  15   5.2   5.0   7.0E-06   1.5E-01
   4  24   4.2   4.4   8.4E-06   1.8E-01
   4  29   5.4   5.4   7.9E-06   1.9E-01
   4  33   4.8   4.8   7.3E-06   1.8E-01
   4  37   6.6   6.8   6.7E-06   1.5E-01
   9  24   4.5   4.5   7.5E-06   2.0E-01
   9  29   4.9   4.9   7.1E-06   1.7E-01
   9  33   4.4   4.3   7.0E-06   1.3E-01
   9  37   5.8   6.0   6.9E-06   1.2E-01
  14  24   3.9   3.9   7.3E-06   1.5E-01
  14  29   4.5   4.5   5.3E-06   1.1E-01
  14  33   3.4   3.4   5.7E-06   1.6E-01
  14  37   3.6   3.6   7.5E-06   1.3E-01
  21   3   4.1   3.9   6.2E-06   1.3E-01
  21   9   4.4   4.4   6.4E-06   1.5E-01
  21  15   4.9   4.9   6.8E-06   1.8E-01
  27   3   4.4   4.4   6.6E-06   1.0E-01
  27   9   4.7   4.6   8.2E-06   1.5E-01
  27  15   5.1   4.9   7.4E-06   2.1E-01
  31   9   4.3   4.3   8.5E-06   1.8E-01
  31  15   4.4   4.4   7.6E-06   1.5E-01
  21  24   4.9   4.9   8.0E-06   1.7E-01
  21  29   5.0   5.0   6.7E-06   1.9E-01
  21  33   4.7   4.7   7.3E-06   1.6E-01
  21  37   4.5   4.5   7.4E-06   1.4E-01
```

```
  27  24   4.8   4.8  7.5E-06  1.8E-01
  27  29   4.4   4.4  7.0E-06  1.3E-01
  27  33   3.8   4.5  7.0E-06  1.7E-01
  27  37   4.1   4.4  7.2E-06  1.2E-01
  31  24   5.3   5.3  7.0E-06  1.8E-01
  31  29   4.4   4.4  6.3E-06  1.4E-01
  31  33   4.2   4.2  6.1E-06  1.3E-01
 1000. 1000. 1000. 1000.
 1000. 1000. 1000. 1000.
     1.  1000.
 -0.10E+21  0.10E-19  2100.  1800.
  0.10E+21  0.30E+01  7200.  4500.
 -0.10E+21  0.10E-19  2100.  1800.
  0.10E+21  0.30E+01  7200.  4500.
 -0.10E+21  0.10E-19  2100.  1800.
  0.10E+21  0.30E+01  7200.  4500.
 -0.10E+21  0.10E-19  2100.  1800.
  0.10E+21  0.30E+01  7200.  4500.
24  300.0  17
0  1  1
3.5622e+07  3.5622e+07  3.5622e+07  3.5622e+07  3.5622e+07
3.5622e+07
3.5622e+07  3.5622e+07  3.5622e+07  3.5622e+07  3.5622e+07
3.5622e+07
3.5622e+07  3.5622e+07  3.5622e+07  3.5622e+07  3.5622e+07
3.5622e+07
3.5622e+07  3.5622e+07  3.5622e+07  3.5622e+07  3.5622e+07
3.5622e+07
3
1.0e-6  0.04  100.
1.0e-6  0.04  100.
1.0e-6  0.04  100.
1.0e-6  0.04  100.
1.0e-6  0.04  100.
1.0e-6  0.04  100.
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1.0e-6  0.04  100.
1.0e-6  0.04  100.
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1.0e-6  0.04  100.
1.0e-6  0.04  100.
1.0e-6  0.04  100.
1.0e-6  0.04  100.
10  15  0.0001905  0.3048  -6.2000  600.0
11  16  0.0001905  0.3048  -6.2006  300.0
11  17  0.0001905  0.3048  -6.2009  300.0
11  18  0.0001905  0.3048  -6.2012  300.0
11  19  0.0001905  0.3048  -6.2015  300.0
11  20  0.0001905  0.3048  -6.2018  300.0
11  21  0.0001905  0.3048  -6.2021  600.0
11  22  0.0001905  0.3048  -6.2027  600.0
```

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10   23   0.0001905   0.3048   -6.2033   300.0
 9   23   0.0001905   0.3048   -6.2036   300.0
 8   23   0.0001905   0.3048   -6.2039   300.0
 7   23   0.0001905   0.3048   -6.2042   300.0
 6   23   0.0001905   0.3048   -6.2045   300.0
 5   23   0.0001905   0.3048   -6.2048   600.0
 4   24   0.0001905   0.3048   -6.2054   300.0
 3   24   0.0001905   0.3048   -6.2057   300.0
 2   24   0.0001905   0.3048   -6.2060   300.0
1  1  1  1
600  1.0  0.005 14.5000  0.0  -0.0  -16.58
8.64e-6  6.1  14.5000  0.0  14.5000  0.0
1000.  14.5000  0.0
0
6
 3   6
 7  12
 9  17
14  19
19  24
24  18
1
7
3
 5   6
14  21
22  18
 0  0  0.  0.  0.      0. 0.   0.   0.    0.    0.
0.  0. 0.  0. 0.
 1   1  -1  14.80  0.  0.  0.
 1   2  -1  14.80  0.  0.  0.
 1   3  -1  14.80  0.  0.  0.
 1   4  -1  14.80  0.  0.  0.
 1   5  -1  14.80  0.  0.  0.
 1   6  -1  14.80  0.  0.  0.
 1   7  -1  14.80  0.  0.  0.
 1   8  -1  14.80  0.  0.  0.
 1   9  -1  14.80  0.  0.  0.
 1  10  -1  14.80  0.  0.  0.
 1  11  -1  14.80  0.  0.  0.
 1  12  -1  14.80  0.  0.  0.
 1  13  -1  14.80  0.  0.  0.
 1  14  -1  14.80  0.  0.  0.
 1  15  -1  14.80  0.  0.  0.
 1  16  -1  14.80  0.  0.  0.
 1  17  -1  14.80  0.  0.  0.
 1  18  -1  14.80  0.  0.  0.
 1  19  -1  14.80  0.  0.  0.
 1  20  -1  14.80  0.  0.  0.
 1  21  -1  14.80  0.  0.  0.
 1  22  -1  14.80  0.  0.  0.
 1  23  -1  14.80  0.  0.  0.
 1  24  -1  14.80  0.  0.  0.
 1  25  -1  14.80  0.  0.  0.
```

1	26	-1	14.80	0.	0.	0.
1	27	-1	14.80	0.	0.	0.
1	28	-1	14.80	0.	0.	0.
1	29	-1	14.80	0.	0.	0.
1	30	-1	14.80	0.	0.	0.
1	31	-1	14.80	0.	0.	0.
1	32	-1	14.80	0.	0.	0.
1	33	-1	14.80	0.	0.	0.
1	34	-1	14.80	0.	0.	0.
1	35	-1	14.80	0.	0.	0.
34	7	-1	13.80	0.	0.	0.
34	8	-1	13.80	0.	0.	0.
34	9	-1	13.80	0.	0.	0.
34	10	-1	13.80	0.	0.	0.
34	11	-1	13.80	0.	0.	0.
34	12	-1	13.80	0.	0.	0.
34	13	-1	13.80	0.	0.	0.
34	14	-1	13.80	0.	0.	0.
34	15	-1	13.80	0.	0.	0.
34	16	-1	13.80	0.	0.	0.
34	17	-1	13.80	0.	0.	0.
34	18	-1	13.80	0.	0.	0.
34	19	-1	13.80	0.	0.	0.
34	20	-1	13.80	0.	0.	0.
34	21	-1	13.80	0.	0.	0.
34	22	-1	13.80	0.	0.	0.
34	23	-1	13.80	0.	0.	0.
34	24	-1	13.80	0.	0.	0.
34	25	-1	13.80	0.	0.	0.
34	26	-1	13.80	0.	0.	0.
34	27	-1	13.80	0.	0.	0.
34	28	-1	13.80	0.	0.	0.
34	29	-1	13.80	0.	0.	0.
34	30	-1	13.80	0.	0.	0.
34	31	-1	13.80	0.	0.	0.
26	1	0	0.	0.	0.	0.
27	1	0	0.	0.	0.	0.
28	1	0	0.	0.	0.	0.
29	1	0	0.	0.	0.	0.
30	1	0	0.	0.	0.	0.
31	1	0	0.	0.	0.	0.
32	1	0	0.	0.	0.	0.
33	1	0	0.	0.	0.	0.
34	1	0	0.	0.	0.	0.
27	2	0	0.	0.	0.	0.
28	2	0	0.	0.	0.	0.
29	2	0	0.	0.	0.	0.
30	2	0	0.	0.	0.	0.
31	2	0	0.	0.	0.	0.
32	2	0	0.	0.	0.	0.
33	2	0	0.	0.	0.	0.
34	2	0	0.	0.	0.	0.
28	3	0	0.	0.	0.	0.
29	3	0	0.	0.	0.	0.

30	3	0	0.	0.	0.	0.
31	3	0	0.	0.	0.	0.
32	3	0	0.	0.	0.	0.
33	3	0	0.	0.	0.	0.
34	3	0	0.	0.	0.	0.
28	4	0	0.	0.	0.	0.
29	4	0	0.	0.	0.	0.
30	4	0	0.	0.	0.	0.
31	4	0	0.	0.	0.	0.
32	4	0	0.	0.	0.	0.
33	4	0	0.	0.	0.	0.
34	4	0	0.	0.	0.	0.
33	5	0	0.	0.	0.	0.
34	5	0	0.	0.	0.	0.
34	6	0	0.	0.	0.	0.
32	32	0	0.	0.	0.	0.
33	32	0	0.	0.	0.	0.
34	32	0	0.	0.	0.	0.
32	33	0	0.	0.	0.	0.
33	33	0	0.	0.	0.	0.
34	33	0	0.	0.	0.	0.
30	34	0	0.	0.	0.	0.
31	34	0	0.	0.	0.	0.
32	34	0	0.	0.	0.	0.
33	34	0	0.	0.	0.	0.
34	34	0	0.	0.	0.	0.
30	35	0	0.	0.	0.	0.
31	35	0	0.	0.	0.	0.
32	35	0	0.	0.	0.	0.
33	35	0	0.	0.	0.	0.
34	35	0	0.	0.	0.	0.
28	36	0	0.	0.	0.	0.
29	36	0	0.	0.	0.	0.
30	36	0	0.	0.	0.	0.
31	36	0	0.	0.	0.	0.
32	36	0	0.	0.	0.	0.
33	36	0	0.	0.	0.	0.
34	36	0	0.	0.	0.	0.
28	37	0	0.	0.	0.	0.
29	37	0	0.	0.	0.	0.
30	37	0	0.	0.	0.	0.
31	37	0	0.	0.	0.	0.
32	37	0	0.	0.	0.	0.
33	37	0	0.	0.	0.	0.
34	37	0	0.	0.	0.	0.
22	38	0	0.	0.	0.	0.
23	38	0	0.	0.	0.	0.
24	38	0	0.	0.	0.	0.
25	38	0	0.	0.	0.	0.
26	38	0	0.	0.	0.	0.
27	38	0	0.	0.	0.	0.
28	38	0	0.	0.	0.	0.
29	38	0	0.	0.	0.	0.
30	38	0	0.	0.	0.	0.

31	38	0	0.	0.	0.	0.
32	38	0	0.	0.	0.	0.
33	38	0	0.	0.	0.	0.
34	38	0	0.	0.	0.	0.
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23	39	0	0.	0.	0.	0.
24	39	0	0.	0.	0.	0.
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28	39	0	0.	0.	0.	0.
29	39	0	0.	0.	0.	0.
30	39	0	0.	0.	0.	0.
31	39	0	0.	0.	0.	0.
32	39	0	0.	0.	0.	0.
33	39	0	0.	0.	0.	0.
34	39	0	0.	0.	0.	0.
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21	40	0	0.	0.	0.	0.
22	40	0	0.	0.	0.	0.
23	40	0	0.	0.	0.	0.
24	40	0	0.	0.	0.	0.
25	40	0	0.	0.	0.	0.
26	40	0	0.	0.	0.	0.
27	40	0	0.	0.	0.	0.
28	40	0	0.	0.	0.	0.
29	40	0	0.	0.	0.	0.
30	40	0	0.	0.	0.	0.
31	40	0	0.	0.	0.	0.
32	40	0	0.	0.	0.	0.
33	40	0	0.	0.	0.	0.
34	40	0	0.	0.	0.	0.
20	41	0	0.	0.	0.	0.
21	41	0	0.	0.	0.	0.
22	41	0	0.	0.	0.	0.
23	41	0	0.	0.	0.	0.
24	41	0	0.	0.	0.	0.
25	41	0	0.	0.	0.	0.
26	41	0	0.	0.	0.	0.
27	41	0	0.	0.	0.	0.
28	41	0	0.	0.	0.	0.
29	41	0	0.	0.	0.	0.
30	41	0	0.	0.	0.	0.
31	41	0	0.	0.	0.	0.
32	41	0	0.	0.	0.	0.
33	41	0	0.	0.	0.	0.
34	41	0	0.	0.	0.	0.
1	36	0	0.	0.	0.	0.
2	36	0	0.	0.	0.	0.
1	37	0	0.	0.	0.	0.
2	37	0	0.	0.	0.	0.
1	38	0	0.	0.	0.	0.
2	38	0	0.	0.	0.	0.
3	38	0	0.	0.	0.	0.

```
 4   38   0   0.   0.   0.   0.
 5   38   0   0.   0.   0.   0.
 1   39   0   0.   0.   0.   0.
 2   39   0   0.   0.   0.   0.
 3   39   0   0.   0.   0.   0.
 4   39   0   0.   0.   0.   0.
 5   39   0   0.   0.   0.   0.
 1   40   0   0.   0.   0.   0.
 2   40   0   0.   0.   0.   0.
 3   40   0   0.   0.   0.   0.
 4   40   0   0.   0.   0.   0.
 5   40   0   0.   0.   0.   0.
 1   41   0   0.   0.   0.   0.
 2   41   0   0.   0.   0.   0.
 3   41   0   0.   0.   0.   0.
 4   41   0   0.   0.   0.   0.
 5   41   0   0.   0.   0.   0.
 0    0    0  0.     0.     0.  0.
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12
 0000.  50000.  50000.  50000.  50000.  50000.
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3
 9   6
14  24
19  17
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1.  1.  1.  1.  1.  1.
1.  1.  1.  1.  1.  1.
0  2.00  0  1  0.30  0.0  0.0  0.0  100.0  40.0  0.0  0.0
1000.  3000.  0.0  0.0
0  0  0.0  0.0  0.0  0.0  0.0
2
0.005  0.001  0.001  0.1
1.00  1.00  1.00  1.00  1.00  1.00
0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
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21.09 21.09 21.09 21.09 21.09 21.09 21.09 21.09
1.00  1.00  1.00  1.00  1.00  1.00
-0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1
-0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1
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1.00  1.00  1.00  1.00  1.00  1.00
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-0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1
200.0
21.09 21.09 21.09 21.09 21.09 21.09 21.09 21.09 21.09
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1.00  1.00  1.00  1.00  1.00  1.00
-0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1
-0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1
200.0
21.09 21.09 21.09 21.09 21.09 21.09 21.09 21.09 21.09
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1.00  1.00  1.00  1.00  1.00  1.00
-0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1
-0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1
200.0
21.09 21.09 21.09 21.09 21.09 21.09 21.09 21.09 21.09
21.09 21.09 21.09 21.09 21.09 21.09 21.09 21.09
1.00  1.00  1.00  1.00  1.00  1.00
-0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1
-0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1
200.0
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-0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1
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200.0
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21.09 21.09 21.09 21.09 21.09 21.09 21.09 21.09
1.00  1.00  1.00  1.00  1.00  1.00
-0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1
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1.00  1.00  1.00  1.00  1.00  1.00
-0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1 -0.1
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21.09 21.09 21.09 21.09 21.09 21.09 21.09 21.09
 4.0   4.0   4.0   4.0   4.0   4.0
 4.00  4.00  4.00
 4.5   4.5   4.5   4.5   4.5   4.5
 4.00  4.00  4.00
 5.0   5.0   5.0   5.0   5.0   5.0
 4.00  4.00  4.00
 5.5   5.5   5.5   5.5   5.5   5.5
 4.00  4.00  4.00
 6.0   6.0   6.0   6.0   6.0   6.0
 4.00  4.00  4.00
 6.5   6.5   6.5   6.5   6.5   6.5
 4.00  4.00  4.00
 7.0   7.0   7.0   7.0   7.0   7.0
 4.00  4.00  4.00
 7.5   7.5   7.5   7.5   7.5   7.5
 4.00  4.00  4.00
 8.0   8.0   8.0   8.0   8.0   8.0
 4.00  4.00  4.00
 8.5   8.5   8.5   8.5   8.5   8.5
 4.00  4.00  4.00
 9.0   9.0   9.0   9.0   9.0   9.0
 4.00  4.00  4.00
 9.5   9.5   9.5   9.5   9.5   9.5
 4.00  4.00  4.00
10.0  10.0  10.0  10.0  10.0  10.0
 4.00  4.00  4.00
10.0  10.0  10.0  10.0  10.0  10.0
 4.00  4.00  4.00
10.0  10.0  10.0  10.0  10.0  10.0
 4.00  4.00  4.00
10.0  10.0  10.0  10.0  10.0  10.0
 4.00  4.00  4.00
10.0  10.0  10.0  10.0  10.0  10.0
 4.00  4.00  4.00
10.0  10.0  10.0  10.0  10.0  10.0
 4.00  4.00  4.00
10.0  10.0  10.0  10.0  10.0  10.0
 4.00  4.00  4.00
10.0  10.0  10.0  10.0  10.0  10.0
 4.00  4.00  4.00
10.0  10.0  10.0  10.0  10.0  10.0
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 4.00  4.00  4.00
10.0  10.0  10.0  10.0  10.0  10.0
 4.00  4.00  4.00
10.0  10.0  10.0  10.0  10.0  10.0
 4.00  4.00  4.00
10.0  10.0  10.0  10.0  10.0  10.0
 4.00  4.00  4.00
3000.0  3000.0  3000.0  3000.0  3000.0  3000.0
3000.0  3000.0  3000.0  3000.0  3000.0  3000.0
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300000.
20.0  20.0  20.0  20.0  20.0  20.0
20.0  20.0  20.0  20.0  20.0  20.0
20.0  20.0  20.0  20.0  20.0  20.0
20.0  20.0  20.0  20.0  20.0  20.0
  3000.0  200000.0  200000.0  200000.0  200000.0   200000.0
200000.0  200000.0  200000.0  200000.0  200000.0   200000.0
200000.0  200000.0  200000.0  200000.0  200000.0   200000.0
200000.0  200000.0  200000.0  200000.0  200000.0   200000.0
3000.  3000.  3000.  3000.  4000.  4000.
4000.  4000.  5000.  5000.  5000.  5000.
6000.  6000.  6000.  6000.  6000.  6000.
6000.  6000.  6000.  6000.  6000.  6000.
0.005  0.001  0.001  0.1
3.4  3.4  3.4  0.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
3.4  3.4  3.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
3.4  3.4  3.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
3.4  3.4  3.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
3.4  3.4  3.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
3.4  3.4  3.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
3.4  3.4  3.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
3.4  3.4  3.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
3.4  3.4  3.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
3.4  3.4  3.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
3.4  3.4  3.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
3.4  3.4  3.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
3.4  3.4  3.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
5.4  5.4  5.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
5.4  5.4  5.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
5.4  5.4  5.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
5.4  5.4  5.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
5.4  5.4  5.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
5.4  5.4  5.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
5.4  5.4  5.4  3.0  1.0  1.0  1.0  1.0  1.0  1.0
1.0  1.0  1.0  1.0  1.0  5.2  5.2  5.2  5.2  5.2  5.2
```

5.4	5.4	5.4	3.0	1.0	1.0	1.0	1.0	1.0	1.0	
1.0	1.0	1.0	1.0	1.0	5.2	5.2	5.2	5.2	5.2	5.2
5.4	5.4	5.4	3.0	1.0	1.0	1.0	1.0	1.0	1.0	
1.0	1.0	1.0	1.0	1.0	5.2	5.2	5.2	5.2	5.2	5.2
5.4	5.4	5.4	3.0	1.0	1.0	1.0	1.0	1.0	1.0	
1.0	1.0	1.0	1.0	1.0	5.2	5.2	5.2	5.2	5.2	5.2
5.4	5.4	5.4	3.0	1.0	1.0	1.0	1.0	1.0	1.0	
1.0	1.0	1.0	1.0	1.0	5.2	5.2	5.2	5.2	5.2	5.2
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

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0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
100.0  100.0  100.0
  2.0    2.0    2.0    2.0    2.0    2.0
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1.75e8  1.75e8  1.75e8  1.75e8  1.75e8  1.75e8
1.75e8  1.75e8  1.75e8  1.75e8  1.75e8  1.75e8
1.75e8  1.75e8  1.75e8  1.75e8  1.75e8  1.75e8
4.0e6  4.0e6  4.0e6  6.0e6  6.0e6  6.0e6
1.0e7  1.0e7  1.0e7  1.0e7  1.0e7  1.0e7
1.5e7  1.5e7  1.5e7  1.5e7  1.5e7  1.5e7
1.5e7  1.5e7  1.5e7  1.5e7  1.5e7  1.5e7
```

APPENDIX A6

MAPS OF REALIZATIONS GENERATED FOR MODEL APPLICATION

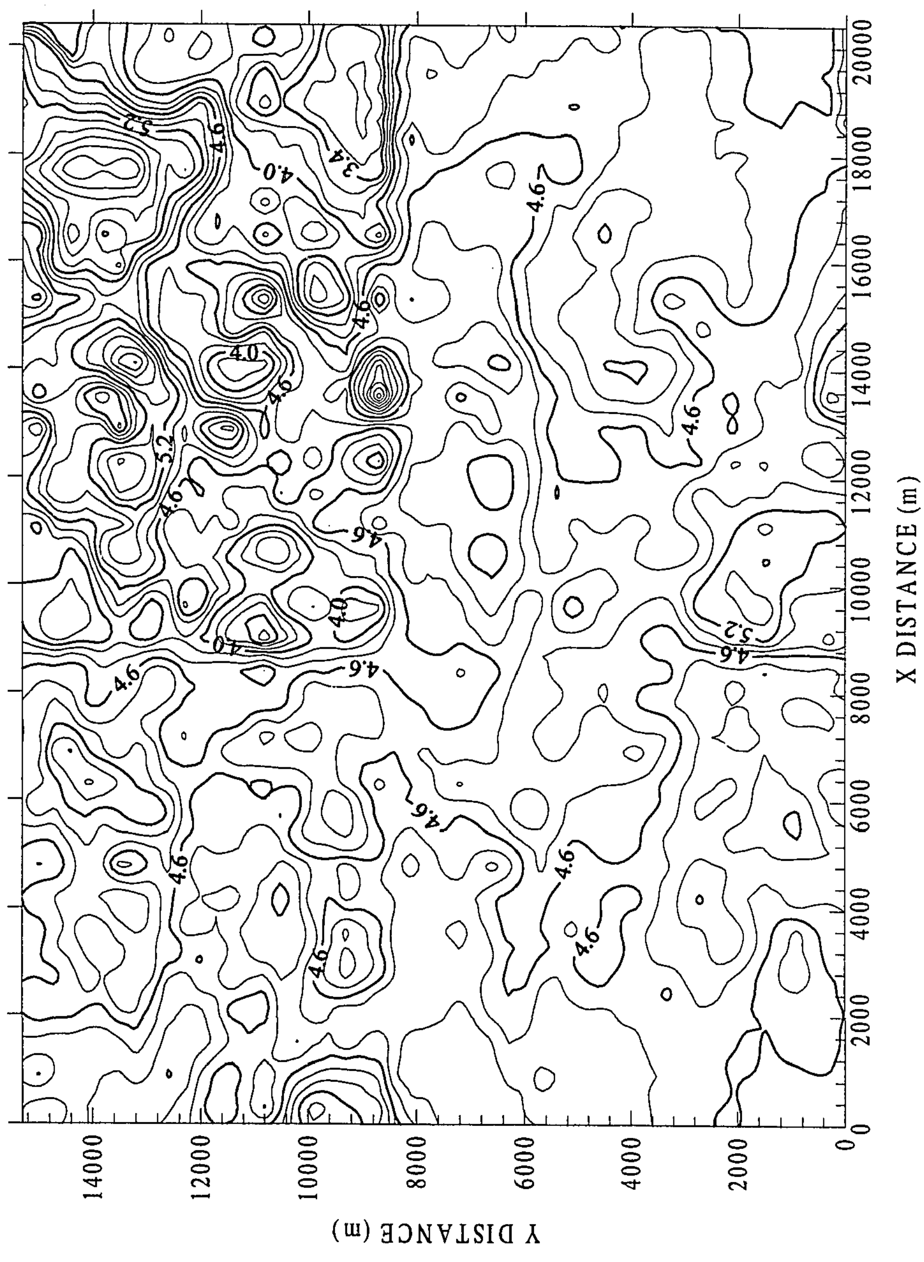

FIG A6.1: MAP OF HYDRAULIC CONDUCTIVITY (m/d) IN X DIRECTION (Realization #2)

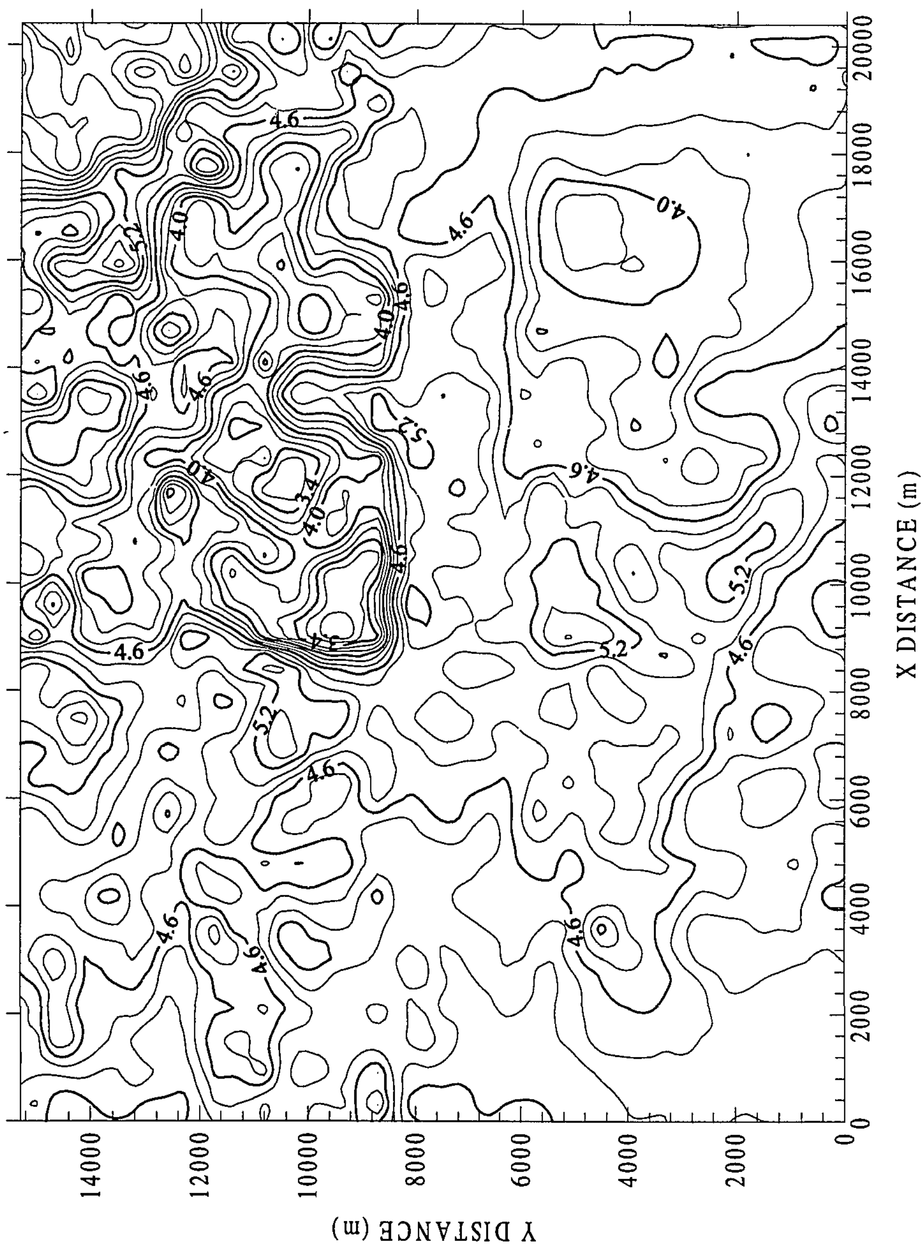

FIG A6.2: MAP OF HYDRAULIC CONDUCTIVITY (m/d) IN X DIRECTION (Realization #3)

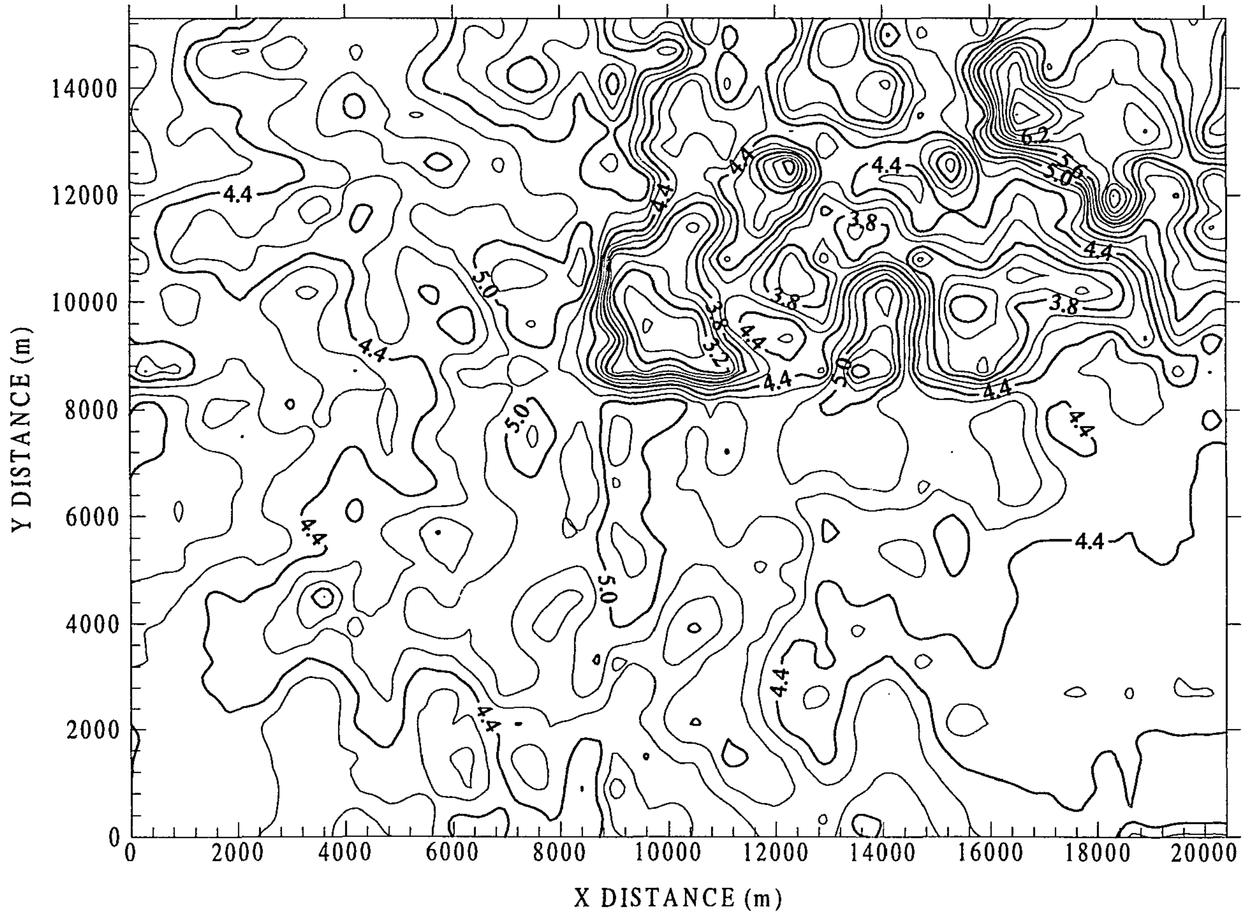

FIG A6.3: MAP OF HYDRAULIC CODUCTIVITY (m/d) IN Y DIRECTION (Realization #3)

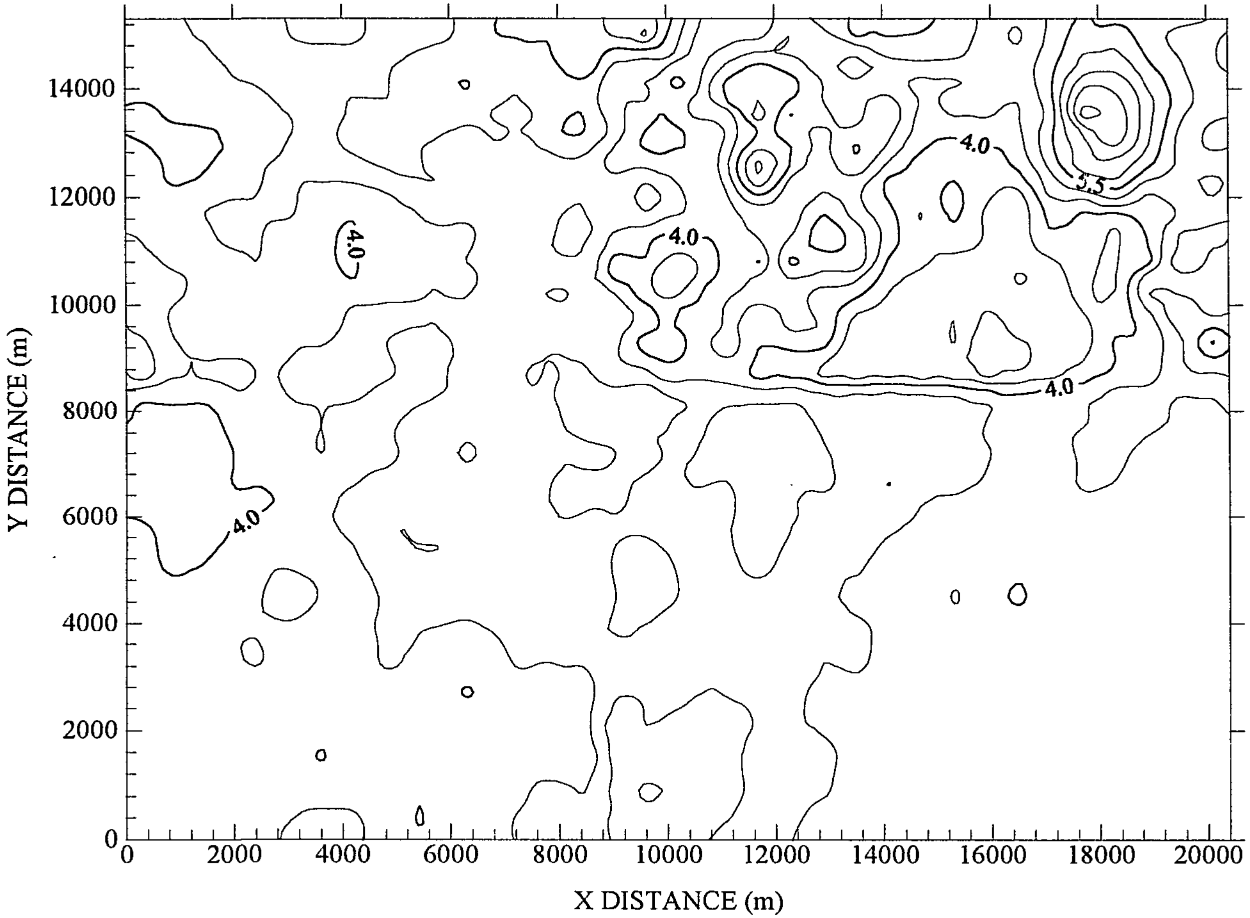

FIG A6.4: MAP OF HYDRAULIC CONDUCTIVITY (m/d) IN Y DIRECTION (Realization #4)

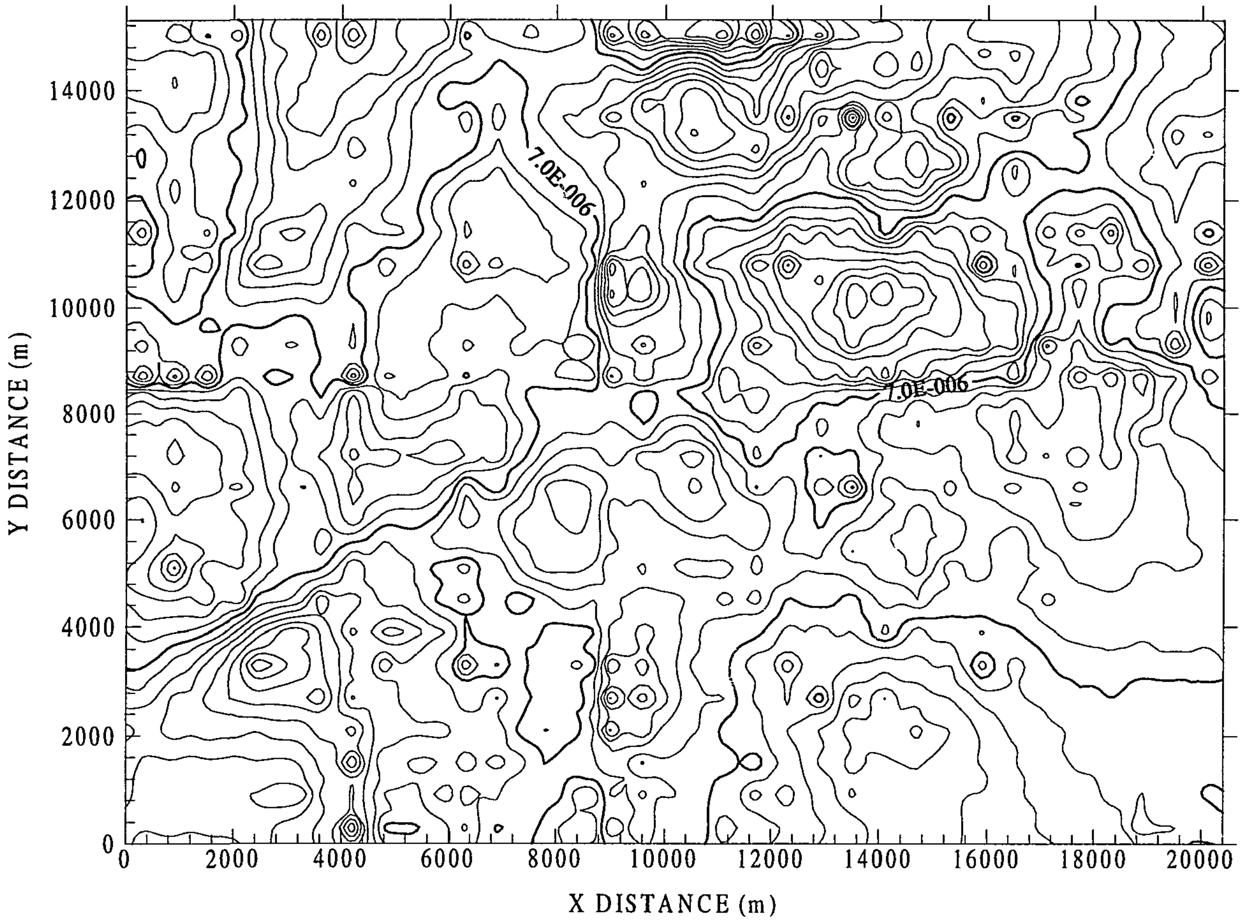

FIG A6.5: MAP OF CONFINED AQUIFER STORAGE COEFFICIENT (Realization #5)