

Optimal Modification of Regional Potentiometric Surface Design for Groundwater Contaminant Containment

Bithin Datta, Richard C. Peralta

ASSOC. MEMBER
ASAE

ABSTRACT

A procedure for optimal modification of a regional potentiometric surface designed solely on the basis of quantitative considerations, is presented. The modification in the potentiometric surface is necessary to incorporate groundwater quality criteria in a critical subsystem of the entire region. The resulting optimal regional potentiometric surface ensures: sustained groundwater yields from the aquifer, compliance with water quality constraints at critical cells of the subsystem (which are identified by a solute transport simulation model), and the most economic conjunctive management of surface and groundwater.

INTRODUCTION

Many methods of developing optimal quantitative water management strategies have been developed (Aquado and Remson, 1974; Alley et al., 1976; Gorelick, 1983). Peralta and Killian (1985) have utilized steady-state flow equations with optimization to develop regional optimal potentiometric surfaces and their attendant conjunctive water use/sustained groundwater withdrawal strategies. Peralta and Peralta, (1984a) had earlier demonstrated that adoption of a sustained yield strategy to maintain 'target' groundwater levels was physically and legally feasible for a critical groundwater use area in Arkansas. We believe that the practice of developing regional sustained yield groundwater withdrawal strategies will increase.

The development of optimal regional potentiometric surfaces and strategies should include consideration of groundwater quality. This is a complex undertaking because of the dependency of contaminant transport on hydraulic stresses and gradients. Louie et al. (1984) has presented one approach of solving this problem by using influence coefficients which describe the effect of regional quantitative groundwater use on regional groundwater quality. Other researchers have demonstrated combined quantitative/qualitative optimization approaches for small hydrologic systems (Molz and Bell, 1977; Remson and Gorelick, 1980; Gorelick and Remson, 1982a,b; Gorelick, 1980; and Gorelick et al., 1979). Several researchers have proposed the use of hydraulic gradient control as a means of preventing contaminant spread by convection (Remson and Gorelick, 1980; Peralta and Peralta, 1984a). Zero or

reverse gradients can easily be imposed as constraints in groundwater management models. There are many cases however, in which some contaminant concentration is acceptable in part of an aquifer. In such situations, the prevention of all convective contaminant movement by rigid gradient control may be overly conservative.

The first purpose of this paper is to describe a procedure for modifying an optimal regional potentiometric surface developed solely with quantitative considerations, in order to satisfy groundwater quality constraints. Although hydraulic gradient control is used within the procedure, it is a flexible control, one that permits groundwater quality to approach, without exceeding, specified limits.

An overview of the procedure is as follows:

1. An optimal regional potentiometric surface and the conjunctive water use/sustained yield strategy that will maintain that surface is developed using the approach of Peralta and Killian (1985).

2. A portion of the region where groundwater quality should be considered is identified as the study subsystem. The steady-state hydraulic stresses that will maintain the groundwater levels within the subsystem in compliance with the optimal regional strategy are determined.

3. The groundwater concentrations resulting from a given optimal regional pumping strategy are determined for the selected subsystem, using a modified form of the two-dimensional solute transport model (Konikow and Bredehoeft, 1978).

4. The computed concentrations are compared with acceptable water use limits.

5. If groundwater quality is unsatisfactory, the change in concentration that will result from any small change in hydraulic head in the selected subsystem is determined. The result is a vector of cell-by-cell influence coefficients.

6. These influence coefficients are used to develop new hydraulic head constraints to be added to the initially used groundwater quantity management model.

7. The modified optimization model is shown to be solvable by using the constrained derivatives for a quadratic optimization model. The modified optimal decision variables include new values of sustained yield groundwater withdrawal which maintain quality criteria imposed on the critical subsystem.

8. Because the influence coefficients used in developing the water quality constraints are not exact, the steady state concentrations resulting from the revised strategy are calculated to verify acceptability. If the water quality results are satisfactory in all cells, the procedure is complete, if not, influence coefficients are calculated for the strategy developed in step 7, and steps 5 to 8 are repeated.

Article was submitted for publication in January, 1986; reviewed and approved for publication by the Soil and Water Div. of ASAE in May, 1986.

The authors are: BITHIN DATTA, post doctorate, and RICHARD C. PERALTA, Associate Professor, Agricultural Engineering Dept., University of Arkansas, Fayetteville.

In order to present the necessary background for explaining the procedure, we discuss two-dimensional groundwater flow and solute transport theory, and finite difference approximations. Adequate discussion of constrained derivatives is also presented.

The second purpose of this paper is to demonstrate the application of the technique to a region in Arkansas. Although the region is one for which several optimal regional sustained yield strategies have been developed (Peralta and Killian, 1985), the groundwater quality problem that is posed is hypothetical. The hypothetical situation presented for the illustrative example is a contaminated canal running along the eastern boundary of the sub-system. Such a situation could be created by the diversion of saline river water through an irrigation canal. The sub-system consists of a township with a potential groundwater contamination problem. The goal is to modify a given optimal steady state groundwater pumping strategy so that the resulting contaminant concentration of groundwater in a particular cell is acceptable.

The main advantage of the proposed procedure is that the influence coefficients are derived directly from the solute transport equation. This eliminates the necessity of making repetitive simulations with a solute transport model, to compute the influence coefficients. In addition, the optimization procedure can be applied even if these influence coefficients are computed by other methods, such as by simulating the changes in concentrations resulting from changes in the hydraulic heads. The approaches presented in Louie et al., (1984), and Gorelick, (1982) are based on simulation of changes in concentrations due to unit changes in pumping values. Our approach does not require these simulations, and is primarily useful for designing an optimal regional potentiometric surface. However, in some cases the proposed method of deriving the influence coefficients directly from the finite difference form of the solute transport equation may prove to be inefficient due to the numerical approximations involved.

GROUNDWATER FLOW EQUATIONS

Transient two dimensional flow of a homogeneous fluid through a non-homogeneous isotropic media can be expressed as:

$$\frac{\partial}{\partial x_i} (T_{ij} \frac{\partial h}{\partial x_j}) = S \frac{\partial h}{\partial t} + W \dots \dots \dots [1]$$

where,

$$W = Q(x,y,t) - \frac{K_z}{m} (H_s - h) \dots \dots \dots [2]$$

- x_i, x_j = cartesian co-ordinates, L
- T_{ij} = transmissivity tensor, L^2T
- h = hydraulic head, L
- S = storage coefficient (dimensionless)
- t = time variable, T
- W = volume flux per unit area (negative for inflow positive for outflow), L/T
- H_s = hydraulic head in the source bed or stream or lake, L
- m = thickness of confining layer, streambed or lake bed, L

- K_z = vertical hydraulic conductivity of stream bed or lake bed
- Q = rate of withdrawal or recharge per unit area (negative for recharge, positive for withdrawal), L/T

For steady state conditions:

$$\frac{\partial}{\partial x_i} (T_{ij} \frac{\partial h}{\partial x_j}) = W \dots \dots \dots [3]$$

A finite difference form of this equation can be found in Konikow and Bredehoeft (1978).

TWO-DIMENSIONAL SOLUTE TRANSPORT AND DISPERSION IN GROUNDWATER

The equation describing the transport and dispersion of a dissolved chemical species can be derived from the principle of conservation of mass in a control volume:

Rate of solute accumulation = (Rate of solute inflow) - (Rate of solute outflow) + (Rate of chemical production by reaction)

This relationship may be expressed mathematically by considering all the fluxes coming in and out of a representative elementary volume of size $\Delta x, \Delta y, \Delta z$; (Konikow and Grove, 1977).

$$\begin{aligned} \frac{\partial}{\partial t} (C \epsilon \Delta x \Delta y \Delta z) = & - \frac{\partial}{\partial x} (C V_x^* \epsilon \Delta y \Delta z) \Delta x \\ & - \frac{\partial}{\partial y} (C V_y^* \epsilon \Delta x \Delta z) \Delta y - \frac{\partial}{\partial z} (C V_z^* \epsilon \Delta x \Delta y) \Delta z \\ & - C^1 W^* \Delta x \Delta y \Delta z + \epsilon \Delta x \Delta y \Delta z \sum_{k=1}^s R_k \dots \dots \dots [4] \end{aligned}$$

Note
 $V^* = \text{sapping velocity}$
 $= \frac{v_{avg}}{\epsilon}$
 $\therefore V^* \epsilon = v_{avg}$
velocity

Where,

- C = concentration of the solute, ML^{-3}
- V_x^*, V_y^*, V_z^* = instantaneous mass velocity of the solute (LT^{-1}) in x, y, and z directions
- $\Delta x, \Delta y, \Delta z$ = dimensions of the control volume, L
- ϵ = effective porosity (dimensionless)
- C^1 = concentration of solute in source or sink fluid, ML^{-3}
- W^* = volume flux per unit volume through a source or sink (positive for outflow, negative for inflow), T^{-1}
- R_k = rate of production of the solute in reaction k of s different reactions (positive for addition of solute, negative for removal), $ML^{-3}T^{-1}$
- b = saturated thickness of the aquifer, L

A particular solute may be added or subtracted from solution within the control volume by chemical reactions, such as radioactive decay, ion-exchange, adsorption etc.

Assuming that the temporal changes in porosity are not significant, and $\Delta x, \Delta y, \Delta z$ are constants, equation [4] can be simplified to the following form:

$$\frac{\partial C}{\partial t} = - \frac{\partial}{\partial x_i} (C V_i^*) - C^1 W^* + \epsilon \sum_{k=1}^s R_k \dots \dots \dots [5]$$

where, i, in x_i and V_i represents the indicial relations of directions (x,y).

The instantaneous mass flux of the solute through a given area. CV_i^* can be separated into two parts.

$$C V_i^* = C V_i + C V_i^1 \dots \dots \dots [6]$$

where,

- V_i^* = instantaneous ^{average} mass velocity of the solute, L/T
- V_i = average interstitial velocity (specific discharge divided by effective porosity) of the fluid, L/T
- V_i^1 = difference between the mass average velocity of solute and the average interstitial (pore) velocity of the fluid (= $V_i^* - V_i$), L/T.

The term (CV_i) represents the convective flux of solute carried by average fluid motion through the elementary volume. CV_i^1 represents the flux caused by hydrodynamic dispersion (resulting from velocity fluctuation or, the deviation of the mass average velocity of the solute from the average velocity of the fluid). Hydrodynamic dispersion denotes the spreading of any solute (at the macroscopic level) resulting from molecular diffusion and mechanical dispersion. Mechanical dispersion is caused by velocity fluctuations in microscopic levels (across any pore cross-section). In groundwater flow problems, diffusive fluxes are generally assumed to be negligible compared to dispersive fluxes. Under this assumption, the coefficient of mechanical dispersion is equivalent to the coefficient of hydrodynamic dispersion. Therefore, the dispersive flux (CV_i^1) can be approximated as:

$$C V_i^1 = -D_{ij} \frac{\partial C}{\partial x_j} \dots \dots \dots [7]$$

D_{ij} = coefficient of mechanical dispersion, L^2T^{-1} .

Equation [7] shows that the dispersive flux is directly proportional to the concentration gradient and its direction is from a higher concentration to a lower concentration.

Substituting the right hand side of equation [7] into equation [6],

$$C V_i^* = C V_i - D_{ij} \frac{\partial C}{\partial x_j} \dots \dots \dots [8]$$

Substituting equation [8] into equation [5], and assuming:

- (a) spatial changes in porosity are negligible
 - (b) a single dissolved chemical species in the flowing groundwater
 - (c) vertical variation in head and concentration are negligible
 - (d) the solute is not affected by chemical reactions
 - (e) the saturated thickness b , is constant over time
- the two-dimensional solute transport equation for groundwater flow may be stated as (Konikow and Bredehoeft, 1978):

$$\frac{\partial C}{\partial t} = \frac{1}{b} \frac{\partial}{\partial x_j} (b D_{ij} \frac{\partial C}{\partial x_j}) - V_x \left(\frac{\partial C}{\partial x} \right) - V_y \left(\frac{\partial C}{\partial y} \right) - \frac{(C^1 - C) W}{\epsilon b} \dots \dots \dots [9]$$

(where $w = W^* \cdot b$)

For steady state conditions i.e., when the concentrations in the aquifer have reached steady magnitudes, $\partial C / \partial t = 0$. Therefore, the left hand side of equation [9] becomes equal to 0. The first term on the right hand side of equation [9] represents the spatial change in concentration due to hydrodynamic dispersion, the second and the third terms show the spatial effect of convective transport, the fourth term represents the effect of a source or sink.

Scheidegger (1961) has shown that for an isotropic aquifer, the dispersivity tensor (D_{ij}) can be defined in terms of two constants, the longitudinal and transverse dispersivities of the aquifer.

The components of the dispersion coefficient (D_{ij}) for two dimensional flow in an isotropic aquifer can be stated as:

$$D_{ij} = \begin{vmatrix} D_{xx} & D_{xy} \\ D_{yx} & D_{yy} \end{vmatrix} \dots \dots \dots [10]$$

where,

$$D_{xx} = \frac{D_L (V_x)^2}{|V|^2} + \frac{D_T (V_y)^2}{|V|^2} \dots \dots \dots [11]$$

$$D_{yy} = \frac{D_T (V_x)^2}{|V|^2} + \frac{D_L (V_y)^2}{|V|^2} \dots \dots \dots [12]$$

$$D_{xy} = D_{yx} = \frac{(D_L - D_T) V_x V_y}{|V|^2} \dots \dots \dots [13]$$

$$|V|^2 = V_x^2 + V_y^2 \dots \dots \dots [14]$$

$$D_L = \alpha_L |V| \dots \dots \dots [15]$$

$$D_T = \alpha_T |V| \dots \dots \dots [16]$$

α_L = longitudinal dispersivity of the aquifer, L

α_T = transverse dispersivity of the aquifer, L

As previously stated, dispersion is a microscopic phenomenon caused by a combination of molecular diffusion and hydrodynamic mixing occurring with laminar flow through porous media. However, the irregular geometries of ground water recharge or discharge, heterogeneity of geological materials, etc., can have more pronounced dispersive effects than microscopic dispersion. As stated in Daly and Morel-Seytoux (1980), 'purely convective processes in homogenous or non-homogeneous media can (also) produce large apparent dispersion'. In a regional study, (where finite difference grid sizes are fairly large) it may be permissible to ignore some of the localized effects of dispersion. Because many complex phenomena affect dispersion, accurate quantitative determination of the dispersion coefficients in an aquifer is difficult. In fact, these coefficients are often treated as fuzzy parameters for calibration.

In our study it was assumed that a small change in the piezometric head in a particular cell (5 km × 5 km)

would not significantly **change** the dispersive portion of the contribution to the steady state concentration.

FINITE DIFFERENCE APPROXIMATION OF THE TWO-DIMENSIONAL SOLUTE TRANSPORT EQUATION

This section describes the development of a finite difference approximation of equation [9], for steady state flow and concentrations. A system of finite difference cells, each five kilometers square was assumed. Each individual cell was considered affected by four neighboring cells and relevant boundary conditions. Coordinates (node) i, j , were assumed to be coincident with the center of a given cell (i, j) .

The velocity in the x direction of ground water flow at the boundary between two nodes (i, j) and $(i+1, j)$, can be computed using Darcy's Law.

$$V_{x(i+1/2,j)} = \frac{K_{xx}(i+1/2,j)}{\epsilon} \left(\frac{h_{i,j} - h_{i+1,j}}{\Delta x} \right) \dots \dots \dots [17]$$

Similar expressions can be derived for velocities in the y -direction. Concentrations at the boundary between the two cells (i, j) and $(i+1, j)$; or (i, j) and $(i, j+1)$ can be interpolated respectively as:

$$C_{i+1/2,j} = \frac{C_{i,j} + C_{i+1,j}}{2} \dots \dots \dots [18]$$

$$C_{i,j+1/2} = \frac{C_{i,j} + C_{i,j+1}}{2} \dots \dots \dots [19]$$

Equation [9] for steady state conditions may now be stated in a finite difference form as:

$$C_{i+1,j} \left[\frac{(D_{xx})_{i+1/2,j}}{\Delta x^2} - \frac{(D_{yx})_{i,j-1/2}}{4 \Delta x \Delta y} + \frac{(D_{yx})_{i,j+1/2}}{4 \Delta x \Delta y} \right] + C_{i,j} \left[\frac{(D_{xx})_{i+1/2,j}}{\Delta x^2} - \frac{(D_{xx})_{i-1/2,j}}{\Delta x^2} - \frac{(D_{yy})_{i,j-1/2}}{\Delta y^2} - \frac{(D_{yy})_{i,j+1/2}}{\Delta y^2} \right] + C_{i-1,j} \left[\frac{(D_{xx})_{i-1/2,j}}{\Delta x^2} - \frac{(D_{yx})_{i,j+1/2}}{4 \Delta x \Delta y} + \frac{(D_{yx})_{i,j-1/2}}{4 \Delta x \Delta y} \right] + C_{i,j+1} \left[\frac{(D_{xy})_{i+1/2,j}}{4 \Delta x \Delta y} - \frac{(D_{xy})_{i-1/2,j}}{4 \Delta x \Delta y} + \frac{(D_{yy})_{i,j+1/2}}{\Delta y^2} \right] + C_{i,j-1} \left[-\frac{(D_{xy})_{i+1/2,j}}{4 \Delta x \Delta y} + \frac{(D_{xy})_{i-1/2,j}}{4 \Delta x \Delta y} + \frac{(D_{yy})_{i,j-1/2}}{\Delta y^2} \right] + C_{i+1,j-1} \left[-\frac{(D_{xy})_{i+1/2,j}}{4 \Delta x \Delta y} - \frac{(D_{yx})_{i,j-1/2}}{4 \Delta x \Delta y} \right]$$

$$+ C_{i-1,j-1} \left[\frac{(D_{xy})_{i-1/2,j}}{4 \Delta x \Delta y} + \frac{(D_{yx})_{i,j-1/2}}{4 \Delta x \Delta y} \right] + C_{i+1,j+1} \left[\frac{(D_{xy})_{i+1/2,j}}{4 \Delta x \Delta y} + \frac{(D_{yx})_{i,j+1/2}}{4 \Delta x \Delta y} \right] + C_{i-1,j+1} \left[-\frac{(D_{xy})_{i-1/2,j}}{4 \Delta x \Delta y} - \frac{(D_{yx})_{i,j+1/2}}{4 \Delta x \Delta y} \right] + C_{i+1,j} \left[-\frac{K_{xx}(i+1/2,j)}{2\epsilon\Delta x^2} (h_{i,j} - h_{i+1,j}) \right] + C_{i,j} \left[-\frac{K_{xx}(i+1/2,j)}{2\epsilon\Delta x^2} (h_{i,j} - h_{i+1,j}) \right] + C_{i,j} \left[+\frac{K_{xx}(i-1/2,j)}{2\epsilon\Delta x^2} (h_{i-1,j} - h_{i,j}) \right] + C_{i,j} \left[-\frac{K_{yy}(i,j+1/2)}{2\epsilon\Delta y^2} (h_{i,j} - h_{i,j+1}) \right] + C_{i,j} \left[+\frac{K_{yy}(i,j-1/2)}{2\epsilon\Delta y^2} (h_{i,j-1} - h_{i,j}) \right] + C_{i-1,j} \left[+\frac{K_{xx}(i-1/2,j)}{2\epsilon\Delta x^2} (h_{i-1,j} - h_{i,j}) \right] + C_{i,j+1} \left[-\frac{K_{yy}(i,j+1/2)}{2\epsilon\Delta y^2} (h_{i,j} - h_{i,j+1}) \right] + C_{i,j-1} \left[+\frac{K_{yy}(i,j-1/2)}{2\epsilon\Delta y^2} (h_{i,j-1} - h_{i,j}) \right] - \frac{(C_{i,j}^1 - C_{i,j}) W_{i,j}}{\epsilon(b)_{i,j}} = 0 \dots \dots \dots [20]$$

Equation [20] can be restated in a matrix form (Gorelick and Remson, 1982a):

$$[D] [C] + [(C^1 - C)W] = [B] \dots \dots \dots [21]$$

- where,
- [D] = a square matrix of finite difference coefficients (size $m \cdot n$ by $m \cdot n$; $m \cdot n$ = total number of finite difference nodes, or cells for a rectangular (or square) system with m rows and n columns)
- [C] = a column vector ($m \cdot n$ by 1) of unknown solute concentrations at every node
- [($C^1 - C$)W] = a row vector ($m \cdot n$ by 1) representing the mass fluxes through the sources and sinks

[B] = a column vector (m·n by 1) of boundary conditions

And standard elimination procedure can be used to solve the system of linear equations (21) to compute steady state concentrations at each node for a given set of hydraulic stresses.

Assuming that the dispersion terms of Equation 20 remain unchanged, the convective and boundary condition terms must be reevaluated in order to compute the steady state concentrations resulting from a small (1% to 5% of the saturated thickness, to ensure only a small change in the transmissivity of the aquifer in a particular cell) change in the hydraulic head ($h_{i,j}$). Also assuming that the aquifer is homogeneous and isotropic with respect to hydraulic conductivity ($K_{xx} = K_{yy} = K$), and that $\Delta x = \Delta y$, Equation 20 may be re-stated as:

$$K_d + K_1 C_{i,j} h_{i,j} + K_2 h_{i,j} + K_3 + K_4 - \frac{(C_{i,j}^1 - C_{i,j}) W_{i,j}}{\epsilon(b)_{i,j}} = 0 \quad \dots \dots \dots [22]$$

where,

$$K_1 = - \frac{2K}{\epsilon \Delta x^2} \quad \dots \dots \dots [23]$$

K_d = sum of all the terms in equation [20] containing the coefficients of dispersion

$$K_2 = - [C_{i+1,j} + C_{i-1,j} + C_{i,j+1} + C_{i,j-1}] \left[\frac{K}{2\epsilon \Delta x^2} \right] \quad \dots \dots \dots [24]$$

$$K_3 = \frac{K}{2\epsilon \Delta x^2} [C_{i+1,j} h_{i+1,j} + C_{i-1,j} h_{i-1,j} + C_{i,j+1} h_{i,j+1} + C_{i,j-1} h_{i,j-1}] \quad \dots \dots \dots [25]$$

$$K_4 = \frac{K}{2\epsilon \Delta x^2} C_{i,j} [h_{i+1,j} + h_{i-1,j} + h_{i,j+1} + h_{i,j-1}] \quad \dots \dots \dots [26]$$

Therefore, for a known set of steady state concentrations computed using any aquifer solute transport model, the assumed constant term K_d can be computed as:

$$K_d = \frac{(C_{i,j}^1 - C_{i,j}) W_{i,j}}{\epsilon(b)_{i,j}} - K_1 C_{i,j} h_{i,j} - K_2 h_{i,j} - K_3 - K_4 \quad \dots \dots \dots [27]$$

After rearranging terms in Equation [22],

$$C_{i,j} = \left(\frac{C_{i,j}^1 - C_{i,j}}{\epsilon(b)_{i,j}} W_{i,j} - K_4 - K_3 - K_d \right) \frac{1}{K_1 h_{i,j}} - \frac{K_2}{K_1} \quad \dots \dots \dots [28]$$

To find the change in concentration in cell (i,j) due to a unit change in $h_{i,j}$ (i.e., determine the influence coefficient at cell (i,j)) Equation [28] can be differentiated with respect to $h_{i,j}$ resulting in:

$$\frac{\partial C_{i,j}}{\partial h_{i,j}} = - \left(\frac{C_{i,j}^1 - C_{i,j}}{\epsilon(b)_{i,j}} W_{i,j} \frac{1}{K_1 (h_{i,j})^2} \right) + \frac{C_{i,j}^1 - C_{i,j}}{\epsilon(b)_{i,j} h_{i,j}} \left(\frac{1}{K_1} \frac{\partial W_{i,j}}{\partial h_{i,j}} \right) + \frac{1}{K_1} \left(\frac{K_d + K_4 + K_3}{h_{i,j}^2} \right) - \left(\frac{\partial K_3}{\partial h_{i,j}} \right) \frac{1}{K_1 h_{i,j}} \left| \begin{matrix} - \left(\frac{\partial K_2}{\partial h_{i,j}} \right) \frac{1}{K_1} \\ \dots \dots \dots \end{matrix} \right|_{h_{i,j}} - \left(\frac{\partial K_4}{\partial h_{i,j}} \right) \frac{1}{h_{i,j} K_1} \left| \begin{matrix} \dots \dots \dots \end{matrix} \right|_{h_{i,j}} \quad \dots \dots \dots [29]$$

where,

$$\left| \begin{matrix} \dots \dots \dots \end{matrix} \right|_{h_{i,j}} = \text{for a given value of } h_{i,j}$$

Note that the concentrations and the volume flux ($W_{i,j}$) are considered as functions of $h_{i,j}$. The hydraulic heads at other cells are assumed to remain constant. The change in $W_{i,j}$ due to a small change in $h_{i,j}$ can be computed by using the finite difference form of the groundwater flow equation (linearized Boussinesq Equation for steady state).

PURPOSE OF SIMULATING AN EQUIVALENT SUB-SYSTEM

The procedure presented in this paper is based on the premise that only a few cells of the entire region are potentially critical in terms of solute concentrations. Therefore, for the sake of computational efficiency, the proposed method need be applied to only a portion of the entire region. First, those cells with potential for exceeding the required limits of concentrations are identified. Then a small sub-system containing those cells is delineated. The boundary conditions and the hydraulic stresses needed to maintain compatibility with a regional steady state withdrawal strategy are determined. As a result, as long as these appropriate boundary conditions and stresses are maintained, the sub-system can be treated independently while developing the concentration influence coefficients. In other words, the solute transport model is applied only to the sub-system.

A modified version of the AQUISIM model (Verdin et al., 1981) is used to determine the equivalent hydraulic stresses (withdrawal and recharge) that must exist in the

subsystem, in order to maintain a predetermined set of hydraulic heads for the cells of the sub-system. These heads are the optimal values obtained from a regional groundwater management model, (such as those discussed in Peralta and Peralta (1984b), Peralta and Killian (1985) or Yazdanian and Peralta (1986)), solved without any quality constraints. Subsequently, the equivalent stresses are used to compute the influence coefficients that reflect the impact of a unit change in the hydraulic head at a given cell in the subsystem, on the resulting steady state concentration at that cell. These influence coefficients are used to formulate new constraints for the previously used optimization model. The modified optimization model can be subsequently used to develop a modified optimal steady state groundwater withdrawal strategy with groundwater quality constraints.

INCORPORATION OF INFLUENCE COEFFICIENTS IN AN OPTIMIZATION MODEL

The following additional constraints are introduced to incorporate quality (concentration) criteria in an optimization model which was initially used for developing a sustained yield groundwater withdrawal strategy without any quality consideration. These constraints are based on concentration influence coefficients calculated using equation [29], and defined as:

$$\frac{\partial C_{i,j}}{\partial h_{i,j}}$$

The new constraints may be stated as:

$$1. C_{i,j} \leq C_{i,j}^u \dots\dots\dots [30]$$

$$2. \bar{C}_{i,j} + (\Delta h_{i,j}) \left(\frac{\partial C_{i,j}}{\partial h_{i,j}} \right) = C_{i,j} \dots\dots\dots [31]$$

$$3. h_{i,j} \leq \bar{h}_{i,j} + \Delta h_{i,j}^{max} \dots\dots\dots [32]$$

$$4. h_{i,j} \geq \bar{h}_{i,j} - \Delta h_{i,j}^{max} \dots\dots\dots [33]$$

$$5. h_{i,j} - \bar{h}_{i,j} = \Delta h_{i,j} \dots\dots\dots [34]$$

The following notation is used.

$\bar{h}_{i,j}$ = initial head (or drawdown) obtained from the solution of the optimization model without any water quality constraints

$h_{i,j}$ = new hydraulic head in cell i,j

$\bar{C}_{i,j}$ = concentration in cell i,j simulated for the initial optimal head distribution

$C_{i,j}^u$ = upper limit on concentration in cell i,j

$\Delta h_{i,j}^{max}$ = maximum allowable change in $h_{i,j}$ determined by the valid range of linear approximation involved in computing the influence coefficient

These constraints are restated in a modified form

following the discussion of constrained derivatives used in solving a quadratic programming problem. Because the objective of the original optimization model involves both volume of groundwater withdrawal and water table elevations as interacting variables (Peralta and Killian, 1985), the objective function is quadratic. All the constraints are linear. This particular model is described following a discussion of the quadratic programming problem and its constrained derivatives. As is shown in a later section, these constrained derivatives can be used directly to find the solution to an optimization model modified to satisfy certain additional constraints.

There are two possible methods of solving the modified optimization model incorporating both groundwater quantity and quality constraints. The first approach is to include the new concentration constraints [30] to [34] in the regional groundwater management model, and solve the new model to determine an optimal regional withdrawal strategy. The second approach is to modify the optimal strategy obtained as a solution to the model without any quality constraints, so that the newly imposed quality constraints and regional optimality conditions are satisfied. The first approach is a standard one. The second approach is much more involved because it requires the use of constrained derivatives to create a modified optimal strategy. However, this particular approach is more efficient for modifying a regional strategy to include additional constraints for a small sub-system of the entire region. Therefore, we will devote the rest of this section to the elucidation of the second approach.

Use of Constrained Derivatives in Solving the Modified Regional Optimization Model

Before discussing the solution of the modified model by using constrained derivatives, it is necessary to clarify the method of solving a quadratic programming problem with the general differential algorithm (Wilde and Brighter, 1967). Much of the discussion in this section is based on Morel-Seytoux (1978).

Assume a quadratic programming (Q.P.) problem with N original variables and K total constraints, which includes K_e original equality constraints. Conversion of the $K - K_e$ inequality constraints into equations requires the incorporation of $K - K_e$ slack variables. This results in $N + K - K_e$ total variables and K equations. Thus the augmented form of the Q.P. problem can be stated as:

$$\text{Min: } Y = \sum_{n=1}^{N+K-K_e} C_n X_n + \frac{1}{2} \sum_{r=1}^{N+K-K_e} \sum_{t=1}^{N+K-K_e} X_r q_{rt} X_t \dots\dots\dots [35]$$

subject to:

$$\sum_{n=1}^{N+K-K_e} a_{kn} X_n = r_k \quad k = 1, K \dots\dots\dots [36]$$

$$\text{and, } X_n^L \leq X_n \leq X_n^U \quad n = 1, N+K-K_e \dots\dots [37]$$

where,

K = total number of constraints

K_e = total number of original equality constraints

N = total number of original variables

- q_{rt} = coefficients of the quadratic terms in the objective function
- C_n = coefficient of the linear terms in the objective function
- a_{kn} = coefficient of the variable X_n in the k -th constraint
- r_k = right hand side of the k -th constraint (a constant)
- X_n^L = lower bound on the variable X_n
- X_n^U = upper bound on the variable X_n

As long as $N > K_e$, there are an infinite number of possible solutions. The purpose of optimization is to select the best solution. One iterative approach to the optimization requires judicious selection of values for $N - K_e$ of the variables in each step. The remaining K variables expressed in terms of the decision variables via the constraint equations, are calculated directly. It is common practice to refer to the $N - K_e$ variables as 'decision' variables and the rest as 'state variables'. Note that the partitioning of the $N + K - K_e$ variables into state and decision variables is transient—it changes with iteration in the search for the optimal solution.

Except for the unusual case of a degenerate solution, the state variables have non-zero values. To solve the Q.P. problem it is necessary to keep track of the correspondence between the original variables and the state or decision variables at every stage of iteration. Necessary variables used for accomplishing this function, and equations necessary to compute the constrained derivatives directly from the coefficients of the objective function and constraints, are discussed in the Appendix. In the Appendix and subsequent equations, superscripts o and n denote beginning and final values, respectively, in an iteration.

The constrained derivatives (V_j) which represent the change in the objective function Y for a given change in the decision variable d_j is defined as:

$$V_j = \frac{\partial Y}{\partial d_j} \quad j = 1, N - K_e \dots \dots \dots [38]$$

It is shown in the Appendix that, in a quadratic programming model, for a given partition between state and decision variables, V_j needs to be calculated only at the first iteration. This is accomplished by using the coefficients in the objective function and the constraints. Therefore, changes in the values of V_j can be easily computed using these coefficients, as long as the partitioning between state and decision variables does not change.

As stated before, for each iterative step (for given partition of the variables), it is possible to define the state variables as functions of the decision variables.

$$S_i = B_i + \sum_{j=1}^{N-K_e} \delta^o_{ij} d_j \dots \dots \dots [39]$$

Therefore,

$$\delta^o_{ij} = \frac{\partial S_i}{\partial d_j} \dots \dots \dots [40]$$

The change in the objective function value associated with a unit change in the state variable S_i (which also

changes the values of the decision variables), can be expressed as:

$$\Delta Y / \Delta S_i = (\partial Y / \partial d_j) / (\partial S_i / \partial d_j) \dots \dots \dots [41]$$

- N = number of original variables
- K_e = total number of equality constraints
- S_i = i 'th state variable
- d_j = j 'th decision variable
- δ_{ij} = decision derivatives of the state variables (constant values for linear constraints)
- B_i = constant term in the linear expression for the i 'th state variable in terms of the decision variables

Once an initial feasible solution has been specified or, a new iteration has been completed, a decision must be made as to whether an optimal solution is attained or, whether a new iteration is to be initiated. The following procedure is used to choose the decision variable to be changed in value, or to be exchanged with a state variable in the search for an optimal solution (equations are given in the appendix).

1. Calculate all V_j $j = 1, N - K_e$
 If all $V_j = 0$; or $V_j < 0$ or > 0 and all corresponding values of d_j have reached either their upper bounds or lower bounds respectively (for minimization), Then Kuhn-Tucker conditions are satisfied and optimal solutions have been reached. Otherwise, step 2 is initiated.

2. It is now required to find:

$$V_{jmax}^+ = \text{Maximum } V_j ; V_j > 0, d_j > d_j^L \dots \dots [42]$$

$$V_{jmax}^- = \text{Maximum } -V_j ; V_j < 0, d_j < d_j^U \dots \dots [43]$$

(The superscripts L and U represent lower and upper bounds respectively.)

The choice of the decision variable candidate for a change and the limit of its change is to be determined by:

- (a) If $V_{jmax}^+ > V_{jmax}^-$, then the most the decision variable $d_{j=p}$ can be decreased is given by, $|\Delta d_p|_{min}$, which is determined by the most restrictive of the following three conditions:
 - (i) the lower bound on the decision variable cannot be violated
 - (ii) the new value of the constrained derivative for that decision variable becomes zero
 - (iii) any one of the current state variables reaches its upper or lower bounds
- (b) If, $V_{jmax}^- > V_{jmax}^+$, it is necessary to increase the value of d_p by $|\Delta d_p|_{min}$ which is again determined by the most restrictive of conditions analogous to to (i), (ii), and (iii).

When condition (iii) is the most restrictive one, the partition between the state and decision variables will change and a state variable will be a candidate for exchanging status with the decision variable. This situation requires further analysis and is an integral part

of the Q.P. optimization algorithm using the general differential method (Morel-Seytoux, 1978). The procedure presented in this paper for modifying a regional pumping strategy (without solving a new optimization model with added constraints) is valid when conditions (i) and (ii) determine the permissible changes. Therefore, we will not go into the details of the case when condition (iii) is most restrictive. Interested readers can refer to Morel-Seytoux (1978) for details.

Any change in the decision variables according to criteria (a) or (b) is possible only at non-optimal points in the solution space, where the Kuhn-Tucker (K-T) conditions are not yet satisfied. However, if some of the variables bounds or the right hand sides of some of the constraints are relaxed, it may be possible to obtain a new optimal solution, by changing one or more of the decision variable values.

In the pumping strategy modification procedure that is presented in this paper, the user has the option of increasing or decreasing the hydraulic head in a single target cell. However, pumpings in cells adjacent to the target cell will change accordingly, to maintain steady state hydraulic conditions. The hydraulic heads in the remaining cells are restricted to the original values, as obtained from the optimal solution to the regional management model without any water quality constraints. However, these drawdowns may be either state or decision variables at the last iteration in the search for a optimal solution to the unmodified model.

If the hydraulic head selected for a change is a decision variable, then the process is simple. By changing the relevant bounds on the decision variable (or relaxing the constraints), it is possible to compute the associated change in the objective function. Again, the most efficient change in the objective function, when one or more constraints are changed, will be the one for the decision variable d_j corresponding to the largest absolute valued V_j . However, if the hydraulic head in the four adjacent cells (according to the adopted finite difference scheme) are restricted to previous optimal values, one must change the pumping values in all five cells to maintain continuity. The change in the objective function, due to a change Δd_j in the hydraulic head at the target cell (a decision variable) can be computed as:

$$\Delta Y = (\partial Y / \partial d_j) \Delta d_j \dots \dots \dots [44]$$

However, if the hydraulic head at a particular cell is a state variable and the related pumping values are decision variables, then:

$$\Delta Y = \sum_{j=1}^5 [(\partial Y / \partial d_j) / (\partial S_i / \partial d_j)] \Delta S_i \dots \dots \dots [45]$$

Here, the new values of the relevant d_j 's are computed directly, by using the finite difference form of the 2-D steady state groundwater flow equation.

Added complications arise when some of the pumping values are state variables and some are decision variables, and the hydraulic head at the target cell is a state variable. In this case the change in the objective function is given by,

$$\Delta Y = \sum_{j=1}^m [(\partial Y / \partial d_j) / (\partial S_i / \partial d_j)] \Delta S_i \dots \dots \dots [46]$$

where, m denotes the number of pumping values which are decision variables out of the total number ($n=5$) of pumping values affected by the cell drawdown at cell (i,j) . Because the rest of the $(n-m)$ pumping values are state variables, they will not influence the objective function, provided they do not violate their upper or lower bounds.

It is reasonable to ascertain whether these changes will satisfy the optimality criteria. First, we consider the case when the hydraulic head at the target cell is a state variable. If the hydraulic head at the target cell is a state variable and its specified bounds are not violated by a desired change, then the resulting solution will still be optimal because the partitioning does not change. If the pumping values affected by the change of head in the target cell are a combination of state and decision variables, then to ensure an optimal solution the relevant state variables should not reach their upper and lower bounds. If the pumping values are all decision variables optimality will be ensured if the hydraulic head at the target cell does not violate its bounds. The second possibility is that the hydraulic head at the target cell is a decision variable. If the hydraulic head at the target cell is a decision variable, the optimality condition is still satisfied as long as the newly imposed bounds on the head at the target cell (Constraints 32-33) are not violated.

There can be another possibility that the newly imposed constraints [30] to [34] cannot be simultaneously satisfied. Therefore, no feasible solution can be obtained with the allowable changes in hydraulic head in the target cell. In that case it is required to solve the optimization model which includes the new constraints imposed on concentrations in the critical cells, and simulate the resulting concentrations to test the validity of the influence coefficients used. If the concentration limits are violated in simulation, the iterative approach of generating new coefficients and then obtaining an acceptable optimal solution is to be repeated, until satisfactory results are obtained.

It should be noted here that the K-T conditions for optimality are satisfied if all the V_j values are equal to zero, or if the decision variables reach their upper or lower bounds. Therefore, consider the modified optimization model that includes concentration constraints [30] to [34]. Even if the newly imposed solutions (after accounting for the head changes) do not result in all V_j equalling zero, the newly imposed constraints (Equation [32]) on the hydraulic heads (and therefore on pumpings) will ensure optimality as long as the state or decision variables do not violate their bounds.

Therefore, it is possible to separate the regional groundwater management model, including the concentration constraints for a sub-system, into two models to be solved sequentially. Model (I) is the original groundwater withdrawal model including all physical constraints, but excluding any qualitative (concentration) constraints. Model (II) is the following optimization model which uses the optimal outputs (h_{ij} obtained from the solution of Model (I); C_{ij} simulated for the target cell using the optimal head distribution obtained from Model (I); and the simulated hydraulic stresses in the sub-system required to maintain the optimal steady state condition in the sub-system. Model

II) can be stated in a mathematical form as:

$$\text{Minimize: } \left| h_{pq} - \bar{h}_{pq} \right| \dots \dots \dots [47]$$

$$\text{Subject to: } C_{pq} \leq C_{pq}^u \dots \dots \dots [48]$$

$$\bar{C}_{pq} + (\Delta h_{pq}) \left(\frac{\partial C_{pq}}{\partial h_{pq}} \right) = C_{pq} \dots \dots \dots [49]$$

$$h_{pq} - \bar{h}_{pq} = \Delta h_{pq} \dots \dots \dots [50]$$

$$\left| h_{pq} - \bar{h}_{pq} \right| \leq \Delta h_{pq}^{\max} \dots \dots \dots [51]$$

$$h_{ij} = \bar{h}_{ij} \quad \text{For } i,j \neq p, q \dots \dots \dots [52]$$

where the target cell is denoted as (i,j=p,q).
 The solution of Model (II) (when solution of Model (I) is used as its input) will be an optimal solution to a model including the original constraints of Model (I), and the concentration constraints [30] to [34]; except when the following condition is not satisfied. The required condition is that the original bounds on the variables (such as hydraulic heads and pumping) are not violated. If these bounds must be violated in order to satisfy the constraints of Model (II), then the partitioning between the state and decision variables at the optimal solution of Model (I) will change. In that case, the entire optimization model (Model (I) with added constraints 30-34) must be solved. A numerical example is presented in the next section to illustrate the aforementioned methodology.

ILLUSTRATIVE EXAMPLE

The regional groundwater management model was applied to an aquifer in the Grand Prairie region of southeastern Arkansas. Most groundwater withdrawal in this area is for agricultural usage. Model (I) (Peralta and Killian, 1985) develops a regional management strategy that minimizes the total cost of conjunctive surface water and groundwater use, subject to the availability of surface water, and the opportunity cost of not producing crops due to the unavailability of water required for irrigation. The objective function of minimizing the total cost is quadratic, because both the static water levels and groundwater withdrawals are decision variables and their product is required to define the dynamic lift in the objective function. Therefore the model has to be solved through the use of a quadratic programming algorithm.

The objective function is to minimize the total cost of water supply:

$$\text{Minimize: } \sum_{k=1}^{nc} P_k \cdot C_{gk} \cdot f(h_k, g_k) + r_k \cdot C_{qk} + u_k \cdot Co_k \dots \dots \dots [53]$$

The constraints are:

1. The finite difference relationship defining steady

state groundwater withdrawal or recharge in a particular cell is a function of average steady state hydraulic head in that cell and the neighbouring cells.

$$P_k + R_k = Q_k = f(h_k) \quad k=1, nc \dots \dots \dots [54]$$

R_k = recharge.

2. Total water supply deficit in a particular cell equals the difference between the supply and demand. The deficit values are used to compute the opportunity cost of deficits in the objective function.

$$P_k + r_k + u_k = w_k \quad k=1, nc \dots \dots \dots [55]$$

Other constraints include: upper and lower bound on pumping in each cell; upper bound on recharge at constant head cells; upper bound on drawdowns for all internal cells; and non-negativity constraint on total water supply deficit in all the internal cells. Details are given in Peralta and Killian (1985).

The following notation is used.

- P_k = groundwater pumping (withdrawal) in cell k, L³
- Q_k = total withdrawal or recharge in cell k (coordinates i,j), L³
- C_{gk} = unit cost of pumping a unit volume groundwater in cell k per unit dynamic head in that cell, \$/L⁴
- h_k = average steady state hydraulic head in cell k (coordinates i,j) measured from an assumed horizontal datum, L
- g_k = distance between the ground surface in cell k (coordinates i,j) and the assumed horizontal datum
- w_k = total water demand in cell k
- $f(h_k, g_k)$ = total dynamic head, a function of static lift, (L)
- r_k = surface water supply in cell k, L³
- C_{qk} = unit cost of surface water supply in cell k, \$/L³
- u_k = deficit of total water supply, i.e., unsupplied portion of total demand in cell k, L³
- Co_k = unit opportunity cost of water supply deficiency in cell k (cost incurred by not utilizing agricultural land due to non availability of irrigation water), \$/L³
- nc = total number of internal cells in the system
- $f()$ = a function of

The finite difference equation defining the pumping in cell k (co-ordinate i,j) as a function of the drawdown in that particular cell and four neighbouring cells are given as (Illangasekare et al, 1984)

$$Q_k = t_{i-1/2,j} h_{i-1,j} + t_{i+1/2,j} h_{i+1,j} - [t_{i-1/2,j} + t_{i+1/2,j} + t_{i,j-1/2} + t_{i,j+1/2}] h_{i,j} + t_{i,j-1/2} h_{i,j-1} + t_{i,j+1/2} h_{i,j+1} \dots \dots \dots [56]$$

Where,

- t_{ij} = transmissivity at the center of the grid i,j
- Subscripts i-1/2, j-1/2 etc. denote values at the

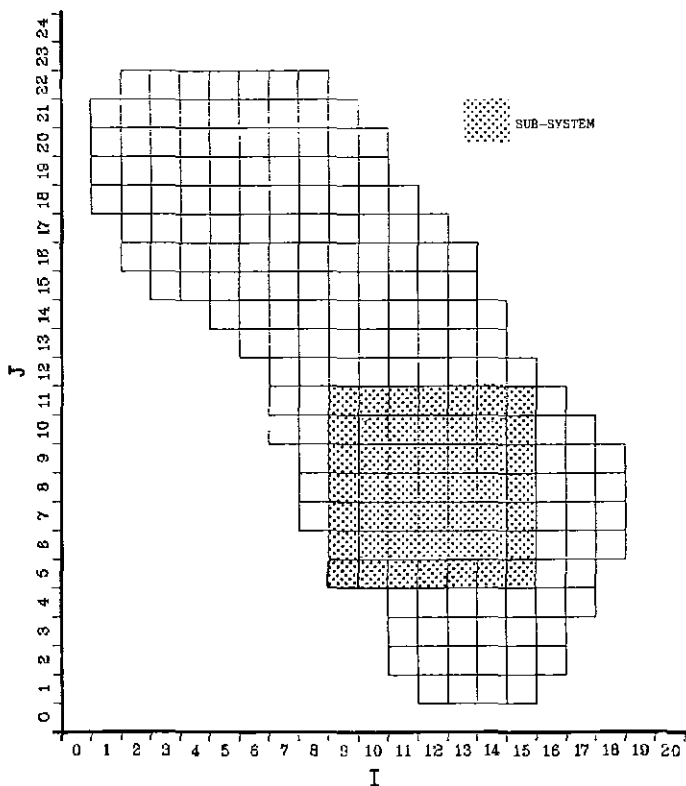


Fig. 1—The entire study area and the sub-system discretized into finite difference cells (5 km × 5 km).

boundary between cells with co-ordinates $i-1$ and i or, $j-1$ and j respectively. These boundary values are the geometric mean of the transmissivities at the center of two neighbouring cells.

Therefore, the optimization model consists of an objective function of minimizing the total cost of conjunctive water use. Other objectives can be included. The constraints imposed include: minimum and maximum pumping based on water needs and diverted surface water availability; minimum allowable saturated

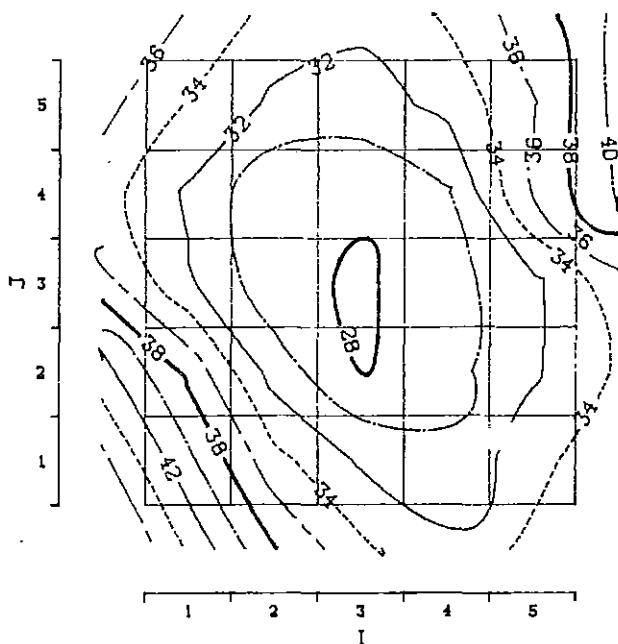


Fig. 2—Contour of optimal hydraulic heads in the sub-system obtained as Model (I) solution (m).

thickness; and upper bounds on recharges at constant-head cells.

Fig. 1 shows a selected sub-system of 49 cells, within the Grand Prairie region. The outermost layer of cells are assumed to constitute a no-flow boundary for the sake of simulating an equivalent hydraulic system, that can maintain a given steady state potentiometric head distribution. In this example, the head distribution is obtained from an optimal solution of Model (I), which does not incorporate any water quality constraints. The next inner layer of cells are considered constant-head cells, and the recharge or discharge through these constant-head cells are assumed equal to the equivalent excitations (discharge or recharge) necessary to maintain the specified head distribution in the sub-system.

The hydraulic heads obtained as optimal values from the optimization model are input to a modified two-dimensional groundwater flow simulation model (AQUISIM; Verdin et al., 1981), to simulate equivalent excitations in the subsystem. The sub-system of cells (excluding the outer most layer), and the contours of steady-state heads obtained as the optimal solution of Model (I) are shown in Fig. 2.

The simulated distributed excitations (pumping in each cell), initial concentration of a single non-reactive contaminant in the aquifer, concentration in recharge or injection (if any), and the aquifer properties are now input to a ground water solute transport model (a modified version of the model developed by Konikow and Bredehoeft, 1978). This model is subsequently used to simulate the steady state concentrations at each cell resulting from the specified optimal hydraulic heads.

We use a modified version of the Konikow and Bredehoeft (1978) transport simulation model to approximately simulate steady-state concentrations. While it may require thousands of years to achieve a steady-state concentration, it is appropriate to look at a limited time horizon (such as 200 years in our case), so that the change in concentration with respect to a single time step is insignificant (close to zero). In our study, the time step is 1 year, and at the end of 200 years of simulation, the yearly changes in concentration are small. Other methods of solving for the steady-state concentrations may require the solution of a set of linear equations (equation [21]), and are more appropriate by some considerations. However, that approach leads one to try to rectify a situation which can arise only after thousands of years. This may not be a desirable approach from a planning perspective.

Fig. 3 shows the sub-system cell numbering system, and the cell-by-cell concentration of the water entering the sub-system through injection or recharge. The steady state concentrations resulting from the equivalent excitations in subsystems are shown in Fig. 4.

The modified solute transport simulation model is capable of computing the influence coefficients which describe the expected change in concentration in any particular cell due to a unit change in the hydraulic head at that cell. These coefficients are now introduced into the optimization model which is modified to include constraints [30] to [34] as quality constraints for the target cell. As discussed before, it is only necessary to find the optimal solution to Model (II) using the optimal solutions of Model (I) as inputs, and then compute the change in the objective function (minimum cost)

j	5	0	0	0	0	1000
		5	10	15	20	25
	4	0	0	0	0	1000
		4	9	14	19	24
	3	0	0	0	0	1000
	3	8	13	18	23	
2	0	0	0	0	0	1000
	2	7	12	17	22	
1	0	0	0	0	0	1000
	1	6	11	16	21	
		1	2	3	4	5
		I				

Fig. 3—Cell numbering in the sub-system and the source concentrations (ppm).

resulting from the changes in the cell variables due to the required change in the hydraulic head in the target cell. The necessary change in the hydraulic head in the target cell is obtained as a solution of Model (II). This procedure will guarantee an optimal solution to the modified optimization model (Model (I) with additional concentration constraints [30-34]), as long as the optimal solution of Model (II) does not change the partition between state and decision variables that existed at the optimality of Model (I).

For the purpose of illustration it is assumed that cell 18 ($i,j=4,3$) is a critical cell with a concentration of 262 ppm. It is required to limit the concentration resulting from a steady state pumping strategy to 235 ppm. The

j	5	0	0	29	115	391
	4	0	0	11	103	195
	3	0	0	43	262	388
	2	0	0	24	234	410
	1	0	0	0	60	224
		1	2	3	4	5
		I				

Fig. 4—Simulated concentrations resulting from the equivalent excitations in the sub-system (ppm).

influence coefficient in this cell is 85.5 ppm/m with allowable range of change in hydraulic head (about 2.0% of the saturated thickness) equal to 0.50 m. This permissible maximum change in hydraulic head is arbitrarily assumed, to ensure that the transmissivity of the aquifer in the target cell does not change more than 2.0% of the value obtained as a solution of Model (I). Otherwise, a significant change in the transmissivity can significantly alter the concentration influence coefficients which are calculated by using the original transmissivities. Therefore for Model (II) the inputs are:

$$\Delta h_{4,3}^{\max} = 0.5 \text{ m}; C_{4,3}^u = 235.0 \text{ ppm};$$

$$\bar{C}_{4,3} = 262.0 \text{ ppm}$$

The necessary change in the hydraulic head in cell number 18 ($i,j=4,3$) to satisfy the concentration constraint in this target cell is 0.3 m. Because the influence coefficient is positive, the hydraulic head has to be decreased in this cell in order to decrease the concentration. The initial optimal value of the cost (solution of Model (I)) is \$9.1 million.

The required change in hydraulic head in this cell will also change the pumping and recharge values in cell numbers 13, 17, 18, 19, and 23, so that a new steady state hydraulic condition can be maintained. The hydraulic head in cell number 18 will decrease by 0.3 m from the value obtained as an optimal solution to Model (I). At the optimality of Model (I) before changing any water levels, the decision variables at the last iteration consisted of the pumping values at cell numbers 13, 18, and 19. All hydraulic heads, and pumping or recharges in all other cells are state variables.

The constrained derivatives with respect to the above mentioned decision variables, change in total cost due to unit change in pumping at the optimality of Model (I) for cells 13, 18, and 19 are—2058.6; 596.7; and 983.7 \$/10⁶ m³ respectively.

The resulting changes in pumping (affected decision variables) due to a 0.3 m decrease in hydraulic head in cell 18 are:

1. Cell number 13, -0.18 million m³/year (decrease)
2. Cell number 18, 0.48 million m³/year (increase)
3. Cell number 19, -0.22 million m³/year (decrease)

The total change in cost due to this revised optimal policy is $[(-2058.6) \times -0.18 + 596.8 \times 0.48 + 983.7 \times (-0.22)]$ or, 3800.0 \$/year. Therefore the total minimum cost for the entire system (204 cells) will be 9,103,800 \$/year compared to 9,100,000 \$/year when no water quality criterion was included. Thus, to meet the new quality constraint in a single cell the modified optimal strategy will cost an additional \$3800.0 annually. It must be noted here that the maximum allowable change in the decision variables (Δd_p), without violating the condition that any of the affected decision variables change into a state variable was also computed. The required changes in the decision variables did not violate this condition. Hence these results are optimal. If any of these limits were violated it would be necessary to resolve the original optimization model with the new constraints using any standard quadratic programming routine.

VALIDATION OF RESULTS

To check the validity of the results, the concentrations in the critical sub-system were again simulated using the modified solute transport model, for the modified water level. For this purpose, the equivalent excitations in the sub-system with a change in water level in cell number 18 were determined using the finite difference equation (equation [55]). The transmissivity values were assumed to remain the same for a small change in hydraulic head at a particular cell.

The new simulated concentration at cell number 18 resulting from a change in hydraulic head of 0.3 m at this particular cell is 232.5 ppm. Therefore the imposed limit of concentration equal to 235.0 is not violated, and the solution of imposing an additional decrease in head of 0.3 m in this cell is acceptable with an appreciable margin of safety. The simulation result also shows that the expected change (obtained from the influence coefficient) in concentration (85.5 ppm/m), is fairly close to the value of 98.5 ppm per m, obtained by simulation.

SUMMARY AND CONCLUSIONS

The methodology discussed here is useful for: (a) simulating the concentration of any single conservative solute contaminant at the nodes of a finite difference grid system which is a subsystem of a larger regional system; (b) determining the influence of a change in an optimal steady-state pumping strategy on steady state concentrations; and (c) modifying a regional optimal steady-state pumping strategy (which was obtained without any quality considerations) to accommodate quality constraints. An added advantage of the procedure is that the influence coefficients are derived directly from a set of specified optimal hydraulic heads. This eliminates the necessity of computing these coefficients by making a separate simulation for each slight variation in assumed hydraulic condition.

The influence coefficients, when incorporated in an optimization model, permit the development of an optimal conjunctive surface water and ground water management strategy that ensures: (a) sustained (steady state) ground water yields from an aquifer; (b) compliance of water quality constraints at critical cells of an aquifer (which are identified by a solute transport model); (c) the most economic conjunctive management of surface and groundwater.

The imposed constraints include: minimum and maximum pumping based on water needs and diverted surface water availability; minimum allowable saturated thickness; recharge limits at constant head cells; and maximum acceptable concentration of a contaminant. The procedure developed also eliminates the necessity of re-resolution of the optimization model when the model is modified to incorporate these additional quality criteria.

Limitations of using this procedure are the approximation involved in computing the influence coefficients, and the assumption that hydraulic heads and concentrations are linearly related through these coefficients (for a small range of change in these heads from a specified value). In its present state of development this procedure is not capable of computing the influences of simultaneous changes in the piezometric heads at all the cells of a subsystem on the concentration at one or more cells. Further study is

necessary to overcome this limitation. However, considering the complexities involved in simultaneously modeling groundwater flow and solute transport while developing an optimal regional pumping strategy, this method is an acceptable approximation.

References

1. Aquado, E. and I. Remson. 1974. Groundwater hydraulics in aquifer management. *Journal of the Hydraulics Division. American Society of Civil Engineers*, 100(HY1), 103-118.
2. Alley, W. M., E. Aquado, and I. Remson. 1976. Aquifer management under transient and steady state conditions. *Water Resources Bulletin* 12(5), 963-972.
3. Beightler, C. S., D. T. Phillips and D. J. Wilde. 1979. *Foundations of optimization*. Prentice-Hall, Englewood Cliffs, N. J.
4. Daly, C. J., and H. J. Morel-Seytoux, 1980. An analytical-numerical procedure for predicting mass transport in groundwater. HYDROWAR Program, CEP80-81CJD-HJM6, Colorado State University, Fort Collins 86p.
5. Gorelick, S. M. 1980. Numerical management models of groundwater pollution. Ph.D. dissertation, Stanford University.
6. Gorelick, S. M., I. Remson and R. W. Cottle, 1979. Management model of a groundwater system with a transient pollution source, *Water Resources Research* 15(5):1243-1249.
7. Gorelick, S. M. 1983. A review of distributed parameter groundwater management modeling methods, *Water Resources Research* 19(2):305-319.
8. Gorelick, S. M., and I. Remson. 1982a. Optimal location and management of waste disposal facilities affecting groundwater quality. *Water Resources Bulletin*, 18(1):43-51.
9. Gorelick, S. M., and I. Remson, 1982b. Optimal dynamic management of groundwater pollutant sources. *Water Resources Research*, 18(1):71-76.
10. Illangasekare, T. H., H. J. Morel-Seytoux and K. L. Verdin. 1984. A technique of reinitialization for efficient simulation of large aquifers using the discrete kernel approach. *Water Resources Research*, 20(11), 1733-1742.
11. Konikow, L. F., and J. D. Bredehoeft. 1978. Computer model for two-dimensional solute transport and dispersion in groundwater. U. S. Geological Survey, *Techniques of Water Resources Investigations*, (7).
12. Konikow, L. F., and D. B. Grove. 1977. Derivation of equations describing solute transport in ground water. U. S. Geological Survey, *Techniques of Water Resources Investigations*, 77-19.
13. Louie, W. F., W. Yeh, and N. S. Hsu. 1984. Multiobjective water resources management planning, *Journal of Water Resources Planning and Management*, ASCE, 110(1), 30-56.
14. Morel-Seytoux, H. J. 1978. *Foundations of engineering optimization*. (bound class notes for CE 620). Dept. of Civil Engineering, Colorado State University, Fort Collins.
15. Peralta, R. C., and P. J. Killian. 1985. Optimal regional potentiometric surface design: least-cost water supply/sustained groundwater yield. *TRANSACTIONS of the ASAE* 28(4):1098-1107.
16. Peralta, R. C. and A. W. Peralta. 1984a. Arkansas groundwater management via target levels. *TRANSACTIONS of the ASAE* 27(6):1696-1703.
17. Peralta, R. C., and A. W. Peralta, 1984b. Using target levels to develop a sustained-yield pumping strategy and its applicability to Arkansas, a riparian right state. Arkansas State Water Plan, Special Report, Arkansas Soil and Water Conservation Commission, Little Rock.
18. Remson, I. and S. M. Gorelick. 1980. Management models incorporating groundwater variables. In *Operations Research in Agriculture and Water Resources*, edited by D. Yaron and C. S. Tapiero, North-Holland, Amsterdam.
19. Scheidegger, A. E., 1961. General theory of dispersion in porous media, *Journal of Geophysical Research*, 66(10), 3273-3278.
20. Verdin, K. L., H. J. Morel-Seytoux and T. H. Illangasekare. 1981. User's manual for AQUISIM: FORTRAN IV programs for discrete kernels generation and for simulation of an isolated aquifer behavior in two dimensions. HYDROWAR Program, Colorado State University, Fort Collins.
21. Wilde, D. J. and C. S. Beightler. 1967. *Foundations of optimization*. Prentice-Hall, Englewood Cliffs, N.J.
22. Yazdani, A., and R. C. Peralta. 1986. Sustained-yield groundwater planning by goal-programming, *Ground Water* 24(2):157-165.

APPENDIX

Equations For Computing The Constrained Derivatives

The objective function (Y) of the Q.P. problem can be stated in terms of the state and decision variables as:

$$Y = \gamma'_s \underline{s} + \gamma'_d \underline{d} + \frac{1}{2} (\underline{s}, \underline{d}) \underline{S} \begin{vmatrix} \underline{s} \\ \underline{d} \end{vmatrix} \dots\dots\dots [A-1]$$

Here, N + K - K_e variables have been partitioned into K state variables and N - K_e decision variables, at a particular iteration.

Or,

$$X = \begin{vmatrix} \underline{s} \\ \underline{d} \end{vmatrix} \dots\dots\dots [A-2]$$

- \underline{s} = column vector of state variables
- \underline{d} = column vector of decision variables
- γ'_s = row vector of coefficients of the linear terms in the objective function (for state variables)
- γ'_d = row vector of coefficients of the linear terms in the objective function (for decision variables)

$$\underline{S} = \begin{vmatrix} S_{ss} & S_{sd} \\ S_{ds} & S_{dd} \end{vmatrix} \dots\dots\dots [A-3]$$

The elements of \underline{S} are the coefficients ($\sigma_{ir}, \mu_{ij}, \kappa_{jt}$) of the quadratic terms in the objective function, when the variables have been partitioned into state and decision variables. The elements of \underline{S} are:

- $S_{ss} = \sigma_{ir}$ (dimension K by K)
- $S_{sd} = \mu_{ij}$ (dimension K by N - K_e)
- $S_{ds} = S_{sd}^{transpose}$ (dimension N - K_e by K)
- $S_{dd} = \kappa_{jt}$ (dimension N - K_e by N - K_e)

Where,

- q(r,t) = coefficients of the quadratic terms in the objective function
- n_s(i) = array of correspondence between the numbering of the original variables and the state variables at a particular iteration (e.g. n_s(4) = 9, denotes that the 9th original variable is the 4th state variable)
- n_s(j) = array of correspondence between the numbering of original variables and the decision variables at a particular stage of iteration
- $\sigma_{ir} = q(n_s(i), n_s(r))$
- $\mu_{ij} = q(n_s(r), n_d(j))$
- $\kappa_{jt} = q(n_d(j), n_d(t))$

It is now possible to state the expression for the constrained derivatives (V_j) which represent the change in the objective function Y for a given change in the decision variable d_j. Using the terms defined earlier, V_j can be defined as:

$$V_j^o = W_j^o + \sum_{t=1}^{N-K_e} T_{jt}^o * d_t \dots\dots\dots [A-4]$$

where,

$$W_j = \gamma_{d_j} + \sum_{i=1}^k \gamma_{s_i} \delta_{ij} + \sum_{r=1}^k B_r (\mu_{rj} + \sum_{i=1}^k \sigma_{ir} \delta_{ij}) \dots\dots\dots [A-5]$$

$$T_{jt} = \kappa_{jt} + \sum_{i=1}^k (\delta_{ij} \mu_{it} + \delta_{it} \mu_{ij}) + \sum_{i=1}^k \sum_{r=1}^k \sigma_{ir} \delta_{ij} \delta_{rt} \dots\dots\dots [A-6]$$

and,

$$T_{jt} = \frac{\partial^2 Y}{\partial d_j \partial d_t} \quad j,t=1, N-K_e \dots\dots\dots [A-7]$$

For quadratic programming, the relationships given by equations [5] and [6] are linear and T_{jt} is a constant as long as the partition between the state and decision variables does not change. Therefore, it is appropriate to use equations [A-5] and [A-6] only at the first iteration for a given partition and then to compute the change in V_j due to any change in a decision variable a, using the following relationship.

$$V_j^n = V_j^o + T_{ja}^o (d_a^n - d_a^o) \dots\dots\dots [A-8]$$

Equations [A-1] to [A-8] provide the necessary relationships for computing the constrained derivatives at the end of a given iteration. Because B_i in equation [39] can be easily computed for a given partition between state and decision variables, equations [A-5] and [A-6] can be incorporated into equations [A-4] or [A-8] to compute the constrained derivatives, solely by using the known coefficients of the objective function. These constrained derivatives are then used to compute the change in the objective function value of Model (I) due to changes in the values of variables as specified by the solution of Model (II).