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REGIONAL TARGET LEVEL MODIFICATION FOR GROUNDWATER QUALITY

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A procedure for modifying an optimal regional potentiometric surface designed solely on the basis of quantitative considerations, is described. These modifications are based on quality considerations in a sub-system of the regional system. The affected changes in the water levels are shown to satisfy optimality criteria under specific conditions. An illustrative example is also provided.

Introduction

Inclusion of groundwater quality considerations in the development of optimal regional strategies is a complex undertaking because of the dependency of contaminant transport on hydraulic stresses and gradients. Louie et. al. (1984) solved 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. An excellent review of some of these approaches is found in Gorelick (1983). 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, 1984). 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 parts 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, which 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 Killián (1985).

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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 steady state groundwater concentrations resulting from the 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 can be derived by using the constrained derivatives for a quadratic optimization model. The modified optimum decision variables include new values of sustained yield groundwater withdrawal which maintain quality criteria imposed within 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.

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, the groundwater quality problem that is posed is hypothetical. A plausible situation for the hypothetical illustrative example is a contaminated canal running along the eastern boundary of the subsystem. 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 contaminant concentration of the groundwater in this particular area is below a specified municipal (or any other) standard.

The main advantage of the proposed procedure for computing the influence coefficients is, that these coefficients are derived directly from the solute transport equation. This method eliminates the necessity of repeated simulations through a solute transport model.

Finite Difference Approximation Of The Two-Dimensional Solute Transport Equation

A finite difference approximation of the two-dimensional groundwater solute transport model for steady state conditions was developed. Finite difference grids, each 5 km (3 miles) square were assumed. Each individual cell was considered affected by four neighboring cells and relevant boundary conditions. Co-ordinates (node) i, j were assumed to be coincident with the center of a given cell (i,j). A detailed discussion of this equation and its finite difference approximation is given in Peralta and Datta (1985).

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

The assumptions used in developing the influence coefficients are as follows. In our study the hydraulic conductivity is assumed homogeneous and isotropic. It was assumed that a small change in the piezometric head in a particular cell (5 km x 5 km) would not significantly change that portion of the steady state concentration contributed by dispersion. Even assuming the dispersion part of the solute transport equation to remain significantly unchanged, the terms describing transport and boundry conditions must still be re-evaluated, in order to compute the resulting steady state concentrations affected by a small (1.0% to 5%) change in the hydraulic head ($h_{i,j}$).

The steady state finite difference form of the solute transport equation can be stated in an expanded form as:

$$C_1 + K_1 C_{i,j} h_{i,j} + K_2 h_{i,j} + K_3 + K_4 - \frac{C^1_{i,j} \cdot W_{i,j}}{\epsilon(b)_{i,j}} = 0 \qquad (1)$$

$$K_1 = -(2 K / \epsilon \Delta x^2) \qquad (2)$$

C_1 = sum of all the terms containing the coefficients of dispersion

$$K_2 = -(C_{i+1,j} + C_{i-1,j} + C_{i,j+1} + C_{i,j-1}) \cdot (K/2\epsilon \Delta x)^2 \qquad (3)$$

$$K_3 = (K/2\epsilon \Delta x^2) \cdot (C_{i+1,j} h_{i+1,j} + C_{i-1,j} h_{i-1,j} + C_{i,j+1} h_{i,j+1} + C_{i,j-1} h_{i,j-1}) \qquad (4)$$

$$K_4 = \frac{K}{2\epsilon \Delta x^2} C_{i,j} (h_{i+1,j} + h_{i-1,j} + h_{i,j+1} + h_{i,j-1}) \qquad (5)$$

Following notation is used.

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

t = time variable

W = volume flux per unit area (positive for inflow negative for outflow)

K = vertical hydraulic conductivity

C = concentration of the solute (ML^{-3})
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 (negative for inflow) (T^{-1})
b = saturated thickness of the aquifer (L)
D = coefficient of dispersion (L^2T^{-1})

Therefore, for a known steady state concentration computed through any aquifer solute transport model, the assumed constant term C_1 can be computed as:

$$C_1 = \frac{C^1_{i,j}\ W_{i,j}}{\epsilon\,(b)_{i,j}} - K_1\, C_{i,j}\, h_{i,j} - K_2\, h_{i,j} - K_3 - K_4 \qquad (6)$$

To find the change in concentration in cell (i,j) due to a unit change in $h_{i,j}$ (= influence coefficient at cell (i,j)). Equation (6) can be differentiated with respect to $h_{i,j}$, so that both 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. Change in $W_{i,j}$, due to small change in $h_{i,j}$, can be computed by using the finite difference form of the groundwater flow equation. Therefore:

$$\partial C_{i,j}/\partial h_{i,j} = -\,(C^1_{i,j}\, W_{i,j}/\epsilon\, b_{i,j})/K_1 \cdot h^2_{i,j} + (C^1_{i,j}/\epsilon\, b_{i,j} \cdot h_{i,j}) \cdot$$
$$(\partial W_{i,j}/\partial h_{i,j})/K_1 + 1/K_1(C_1 + K_3 + K_4)/h^2_{i,j} - (\partial K_3/\partial h_{i,j})/(K_1\, h_{i,j})$$
$$-\,(\partial K_2/\partial h_{i,j})/K_1 - \partial K_4/\partial h_{i,j}(1/h_{i,j})/K_1 \qquad (7)$$

Simulation Of An Equivalent System

The procedure presented in this paper is based on the premise that only a subsystem of the entire region is potentially critical in terms of solute concentrations. Therefore, is is appropriate to identify those cells with potential for exceeding the desirable concentration limits, and group these cells into a small subsystem of the regional system. If the hydraulic stresses and boundary conditions are simulated, so that this subsystem can be treated independently for the purpose of developing the concentration influence coefficients, then the solute transport model is to be applied to only a small subsystem rather than the entire region. Note that the assumptions made in the finite difference approximations implicitly discount the influence of hydraulic stresses at far away cells, on a particular cell.

A modified version of the AQUISIM model (Verdin et. al., 1981) is used to simulate the equivalent hydraulic stresses (withdrawal and recharge) in a subsystem, that will maintain initially obtained steady state hydraulic heads at all cells of the sub-system. The initial heads were the optimal values obtained from a regional groundwater management model, which was solved without any contamination constraints. Subsequently, these equivalent stresses for the subsystem 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, in order 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 in an optimization model to incorporate quality (concentration) criteria in a regional conjunctive surface water and groundwater management strategy. These constraints are based on concentration influence coefficients defined as: $(\partial C_{i,j} / \partial h_{i,j})$. The new constraints may be stated as:

1. $C_{i,j} \leq C^*_{i,j}$ (8)
2. $\bar{C}_{i,j} + \Delta h_{i,j} \cdot \left(\frac{\partial C_{i,j}}{\partial h_{i,j}}\right) \leq C^*_{i,j}$ (9)
3. $h_{i,j} \leq \bar{h}_{i,j} + \Delta h^{max}_{i,j}$ (10)
4. $h_{i,j} \leq \bar{h}_{i,j} - \Delta h^{max}_{i,j}$ (11)
5. $h_{i,j} - \bar{h}_{i,j} = \Delta h_{i,j}$ (12)

$\bar{h}_{i,j}$ = initial head (or drawdown measured from a datum) obtained from the solution of the optimization without any water quality constraints.
$\bar{C}_{i,j}$ = concentration simulated from initial optimal strategy

$C^*_{i,j}$ = upper limit on concentration in cell i,j

$\Delta h^{max}_{i,j}$ is determined by the valid range of linear approximations involved in computing the influence coefficients.

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: $V_j = (\partial Y / \partial d_j)$ (13)

It can be shown that, a quadratic programming model must calculate V_j only at the first iteration of a particular partition between state and decision variables. V_j is calculated using the coefficients of the objective function and the constraints. Changes in these constrained derivatives at successive iterations can be easily computed once the optimal allowable changes in the decision variable values have been determined. A detailed description of the constrained derivatives and their application to constraining groundwater contaminant movement are given in Peralta and Datta (1985).

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: i) the original groundwater withdrawal model including all physical constraints, and excluding any quality (or concentration); and ii) the following optimization model which uses the optimal $\bar{h}_{pq}$ output from the quantative model, and the resulting simulated $\bar{C}_{pq}$; for i,j≠p,q.

Minimize: $\left| h_{pq} - \bar{h}_{pq} \right|$ subject to the constraints 8 to 12 and the additional constraint: $[h_{ij}] = \bar{h}_{ij}$ For $i,j \neq p,q$ (14)

In general an optimal solution to this modified model based on the output from the original management model without any concentration constraints will be an optimal solution to a model including the original constraints and the concentration constraints. The exception is the unlikely case in which the drawdowns at cells $i,j = p,q$: and the related pumping values are all state variables at the optimality of the original model. A necessary criterion for the modified strategy to be an optimal strategy is that the original bounds on the variables (such as hydraulic heads and pumping) are not violated. If in order to satisfy the new constraints these bounds are needed to be violated, then the partitioning between the state and decision variables will have to change, and the entire optimization model with concentration constraints will need to be solved again. However, because the influence coefficients are determined external to the optimization model for specific optimal hydraulic heads, an iterative procedure to recalculate the influence coefficients, is to be initiated in such a situation. A numerical example is presented in the next section to illustrate the methodology discussed so far.

Illustrative Example

The regional groundwater management model was applied to an aquifer in the Grand Prairie Region of south east Arkansas. The major portion of the groundwater withdrawal is for agricultural usage. The objectives of the model (Peralta and Killian, 1985) is the minimization of 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 unavailibility of water required for irrigation. The objective function of minimizing the total cost of conjunctive ground and surface water use is quadratic, because both the groundwater levels and groundwater withdrawals are decision variables and their product is used to estimate the cost of groundwater in the objective function. Therefore, the model is solved through a non-linear quadratic programming algorithm, as detailed in Peralta and Killian (1985).

The model constraints include:

1. The finite difference relationship defining steady state groundwater withdrawal or recharge in a particular cell as a function of average groundwater level in that cell and the neighboring cells.
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.

Other constraints include: upper and lower bound on pumping in each cell; upper bound on recharge at constant head cells; upper bound on water levels for all internal cells; and non-negativity constraint on total water supply deficit in all the internal cells.

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 neighboring cells is given by Illangasekare and Morel-Seytoux (1980); and Peralta and Killian (1985).

A subsystem of 49 cells, which belong to a regional system of 204 cells, is considered critical in terms of groundwater quality criteria. The outermost layer of cells are assumed to constitute a no-flow boundary in the model used for simulating an equivalent hydraulic stresses, that maintain a given steady state piezometric head distribution. These head distributions are obtained from an initial solution of the optimization model without any water quality constraints. The next layer of cells are considered constant head cells without any constraints on the amount of recharge.

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.

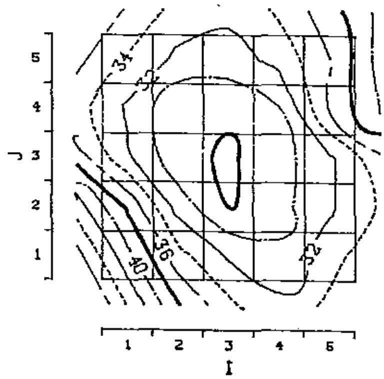

Figure 1. Contour of piezometric heads in the sub-system

	1	2	3	4	5
5	5	10	15	20	25
	0	0	29	115	391
4	4	9	14	19	24
	0	0	11	103	195
3	3	8	13	18	23
	0	0	43	262	388
2	2	7	12	17	22
	0	0	24	234	410
1	1	6	11	16	21
	0	0	0	60	224

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Figure 2. Cell numbering system and simulated concentrations resulting from implementation of unmodified regional strategy

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 then input to a groundwater solute transport model (a modified version of the model developed by Konikow and Bredehoeft, 1978). Figure 1 shows the cell sub-system with the piezometric heads obtained from the initial optimization model. The steady state concentrations resulting from the steady state pumping strategy are shown in Figure 2. This model is now used to simulate the steady state concentrations at each cell resulting from the given optimal drawdowns or piezometric heads. This modified model is capable of computing the influence coefficients that show the expected change in the steady state concentration in any particular cell due to a unit change in the water level at that cell. These coefficients are now introduced into the modified optimization model incorporating quality constraints. However, as discussed before, except for some special cases, it is sufficient to compute the change in the original objective function and the changes in the cell variables caused by the required change in the hydraulic head in a particular cell, which has been identified as a critical one. This procedure will guarantee an optimal solution to the original optimization model, with the second optimization model for the subsystem embedded as a secondary model, so long the partitioning between the state and decision variables of the original model are not forced to change due to the additional criteria set by the secondary model.

For the purpose of illustration it is assumed that cell 18 (i,j = 4,3) is a critical cell with a concentration of 262ppm. It is required to limit the concentration resulting from a steady state pumping strategy to 235ppm. The influence coefficient in this cell is 85.5ppm per m, with allowable range of change in drawdown (about 2.0% of the saturated thickness) equal to 0.50 m. Therefore, for the secondary model, the inputs are: $\Delta h^{max}_{4,3} = 0.5$ m; $C^{*}_{4,3} = 235$ppm; $\bar{C}_{4,3} = 262$ppm.

The required change in the drawdown in cell number 18 (i,j=4,3) is 0.3 m. Because the influence coefficient is positive, the hydraulic head must be decreased in this cell, in order to decrease the concentration. The initial optimal value of the cost is $9.1 million.

The required change in water level in this cell affects the pumping and recharge values in cell numbers 13, 17, 18, 19, and 23. The new value of water level in cell number 18 will be 62.5 m (62.2 + 0.3) from a datum 91.4 m above sea level. It is found that at the original optimality the decision variables at that stage of iteration consist of the pumping values at cell numbers 13, 18, and 19. All water level values and pumping or recharges in all other cells are state variables. The constrained derivatives with respect to these decision variables are given as: change in total cost due to unit change in pumping in cells 13, 18, and 19 are, - 2058.6; 596.7; and \$983.7 $\$/10^6$ m^3 respectively.

The resulting changes in pumping (affected decision variables) due to change in water level in cell 18 are:

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

The total change in cost due to this revised optimal policy is
(-2058.6) * -0.18 + 596.8* 0.48 + 983.7 * (-0.22) = 3800.0 $/year.
Therefore, the total minimum cost for the entire system (204) cells is 9.1038 million $/year compared to 9.1 million $/year cost 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 change in the decision variables $(\Delta d_p)_s$ allowable without violating the condition that any of the affected decision variables change into state variable is also computed. The required changes in the decision variables do 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.

1m=3.28 ft; 1 cubic m = 35.3 cubic ft.

Validation of Results

To check the validity of the results, the concentrations in the aquifer were again simulated using the solute transport model. For this purpose, the equivalent excitations in the sub-system with modified water level in cell number 18 was again simulated using the modified AQUISIM model. It should be noted here that the new excitation (pumping) value for cell number 18 was computed by a finite difference equation defining the pumping in a cell as a function of the water levels in the four neighboring cells(for computing influence coefficients).

The new simulated concentration at cell number 18 resulting from a change in head of 0.3 m at this particular cell is 232.5ppm. Therefore, the imposed limit of concentration equal to 235ppm is not violated, and the solution for decreasing the water level by 0.3 m in this cell is acceptable with some safety margin. The simulation result also shows that the expected change (obtained from the influence coefficient) in concentration (85.5), is fairly close to the value of 98.5, obtained by simulation. Other cases have also been tested for validation.

Summary And Conclusions

The methodology discussed here, is useful for: 1) 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; 2) determining the influence of a change in an optimal steady state pumping strategy on steady state concentrations; 3) modifying a steady state optimal pumping strategy with various quantity and quality constraints, to accomodate quality considerations. An added advantage of the procedure presented here, is that the influence coefficients are derived directly from a set of specified optimal drawdown values. This eliminates the necessity of computing these coefficients through subsequent simulations with changed hydraulic conditions.

The influence coefficients, when incorporated in an optimization model, permit the development of an optimal conjunctive surface water and groundwater management strategy that ensures: 1) sustained (steady state) groundwater yields from an aquifer; 2) compliance of water quality constraints at critical cells of an aquifer (which are identified by a solute transport model); 3) the most economic conjunctive management of surface and groundwater.

This procedure relies on the validity of 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. This procedure, in its present state of development 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. We are in the process of developing a method to overcome this limitation. However, given the complexities involved in the simultaneous modeling of groundwater flow and solute transport in an aquifer, to develop an optimal regional pumping strategy, this method can be an acceptable approximation.

Appendix 1 - References

1. Gorelick, S. M., 1983. A review of distributed parameter groundwater management model methods. Water Resources Research, 19(2), 305-319.

2. Illangasekare, T. and Morel-Seytoux, H. J., 1980 . A technique of re-initialization for efficient simulation of large aquifers using the discrete kernel approach. Unpublished, Hydrowar Program, Colorado State University, Fort Collins.

3. Konikow, L. F., and Bredehoeft, J. D. 1978. Computer Model for two-dimensional solute transport and dispersion in ground water, U.S. Geological Survey, Techniques of Water Resources Investigations, 7.

4. Louie, W. F., Yeh, W. W. G., and Hsu, N. S., 1984. Multiobjective Water Resources Management Planning, Journal of Water Resources Planning and Management, A.S.C.E., 110(1), 39-56.

5. Peralta, R. C. and Killian, P., 1985. Optimal regional potentiometric surface design, least-cost conjunctive water use/sustained groundwater yield. In review, for publication in the Transactions of the American Society of Agricultural Engineers.

6. Peralta, R. C. and Peralta, A. W., 1984. Arkansas Groundwater management via target level. Transactions of the American Society of Agricultural Engineers, vol. 27, No. 6.

7. Remson, I., and Gorelick, S. M., 1980. Management models incorporating groundwater variables, in Operations Research in Agricultural and Water Resources, edited by D. Yaron, and C. S. Tapiero, North Holland Amsterdam.

8. Peralta, R. C., and Datta, B., 1985. Optimal modification of regional potentiometric surface design for groundwater contaminant containment, submitted for publication in: Transactions of the American Society of Agricultural Engineers.

9. Verdin, K. L., Morel-Seytoux, H. J. and Illangasekare, T., 1981. User's Mannual for AQUISIM, HYDROWAR program, Colorado State University, Fort Collins.