DEVELOPMENT OF A COMBINED QUANTITY AND QUALITY MODEL

FOR

OPTIMAL UNSTEADY GROUNDWATER MANAGEMENT

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ABSTRACT

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Presented are alternative techniques for including conservative solute transport within computer models for optimizing groundwater extraction rates. Unsteady two-dimensional flow and dispersed conservative solute transport are assumed. Comparisons are made of the practicality of including modified forms of implicit and explicit finite difference solute transport equations within optimization models. These equations can be calibrated and subsequently used within a MODCON procedure. The MODCON modelling procedure consists of an integrated series of five optimization or simulation modules. The procedure is applicable for either an entire aquifer system or for a subsystem of a larger system. The first module, A, computes physically feasible recharge rates across the boundaries of the modelled subsystem. Module B computes optimal extraction rates without considering groundwater quality. Module C uses method of characteristics simulation to compute solute transport that would result from implementing the pumping strategy of model B. Module D uses linear goal programming and nonlinear solute transport equations to calibrate linear coefficients. It attempts to duplicate the solute transport predicted by module C. Calibration is performed because coarsely discretized implicit or explicit solute transport equations may not be as accurate as the method of characteristics. Module E includes appropriate calibrated equations of module D as well as the flow equations of module B. It computes an optimal pumping (extraction or recharge) strategy that can satisfy future groundwater contaminant concentration criteria. Testing of the validity of this optimal pumping strategy is subsequently accomplished using module C. If necessary, one may cycle through modules C, D and E until convergence is obtained--until concentrations resulting from implementing the strategy of E are demonstrated to be acceptable.

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INTRODUCTION

A. Purpose and Objectives

Assuring the sustainable availability of groundwater for water users requires consideration of both quantitative and qualitative issues. Numerous computer models have been reported for optimizing the quantitative use of groundwater. Far fewer models include solute transport. Most of those are appropriate for injection of contaminated water, because in that case the mass flux rate at injection wells can be considered as a single variable. Optimizing groundwater extraction rates if groundwater quality is unknown is less frequently done (except through gradient-control methods). This reluctance results from the fact that solute transport equations are nonlinear. The use of nonlinear constraints in optimization models results in locally rather than globally optimal solutions. For some management objectives, local optimality is acceptable. This report discusses such a scenario.

The primary purpose of this report is to demonstrate how a linked sequence of five optimization, calibration and simulation models (modules) can be used to develop optimal groundwater management strategies that appropriately consider groundwater quality. To accomplish this we present an enhanced version of the MODCON methodology presented by Peralta et al (1987). The first

objective is to demonstrate the practicality of using calibrated explicit solute transport equations within MODCON to solve a hypothetical problem. The second objective is to compare explicit and implicit versions of MODCON.

B. Related Research and Activities

Gorelick (1983) provides a review of methods for representing solute transport within optimization models. Each method has limitations. Several researchers, including Gorelick (1984) have used nonlinear constraints to represent solute transport. This is done because both extraction rates and the concentration of the extracted water are unknown. A weakness of using nonlinear constraints is the difficulty in assuring global optimality of the computed solutions.

A second approach to managing groundwater concentrations is to use gradient control or velocity influence coefficients (Colarullo et al., 1984; Gorelick and Lefkoff, 1985). This approach may be unnecessarily restrictive if some contaminant movement (in addition to that caused by dispersion) is acceptable. Using predetermined limits on acceptable hydraulic gradients may also be somewhat impractical if the region of contamination is large.

A third method utilizes influence coefficients that describe the effect of a change in potentiometric head on steady-state

concentractions (Datta and Peralta, 1986). This approach is overly restrictive since steady-state concentrations do not usually occur rapidly. It is also cumbersome and impractical if concentrations must be managed at multiple locations.

Another influence coefficient approach is described by Louie et al., (1984). It does not include detailed simulation of transport processes and may be impractical if concentrations must be managed at numerous locations simultaneously.

Peralta et al (1987) demonstrate use of linear mass transport equations within two-dimensional models for optimizing groundwater management. These equations utilize linear coefficients calibrated to approximately represent the solute transport that is predicted using method of characteristics (MOC) simulation. They use a MODCON procedure consisting of five linked modules. Their computed optimal pumping strategy does cause an acceptable reduction in future concentrations at target cells. However, the accuracy of the solute transport equations was unsatisfactory. One would expect a repetitive cycle of calibration, optimization, simulation, calibration, etc., to cause concentrations predicted by the optimization model to converge to those predicted by the simulation model. This did not occur.

This paper reports testing performed using significantly modified MODCON modules. Described changes result in enhanced

simulation of solute transport. Although linear coefficients are still utilized, nonlinear solute transport equations are used as constraints. As a result, computed strategies are locally, not necessarily globally, optimal. Another enhancement to the previously reported MODCON procedure is the coding of MOC solute transport using GAMS/MINOS, permitting more rapid interaction between modules. In the previously reported MODCON, MOC simulation was accomplished using an external FORTRAN simulation model.

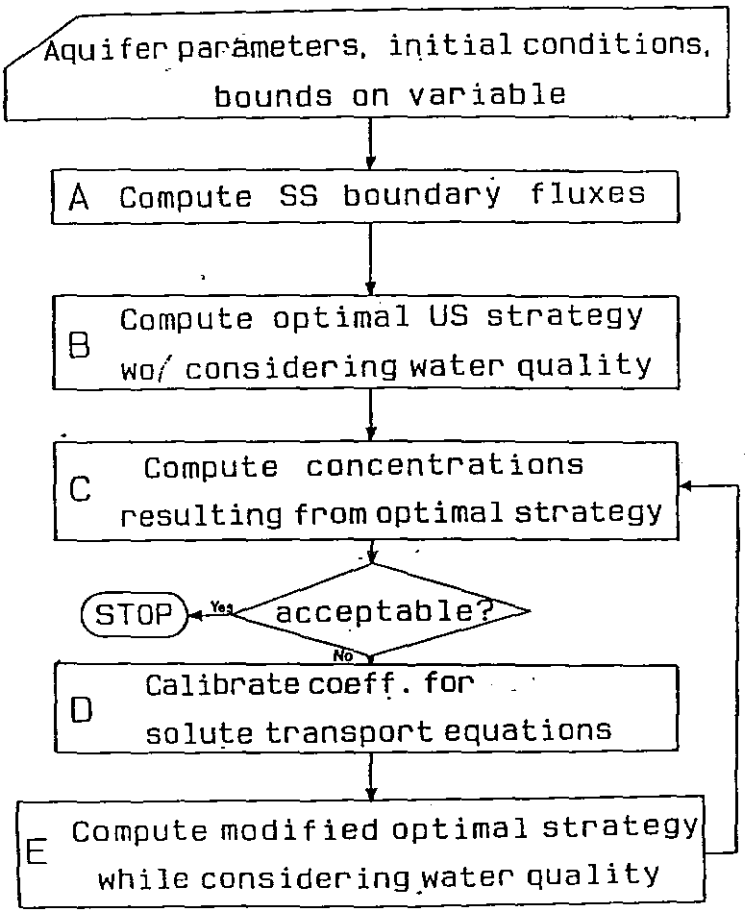
METHODS AND PROCEDURES

A. Modelling Methodology Overview and Functions

We assume: 1) an unconfined isotropic heterogeneous aquifer in which the change in water levels with time will cause insignificant change in transmissivity (although anisotropic hydraulic conductivity can be readily considered, isotropic conductivity is used here), 2) two-dimensional unsteady groundwater flow, 3) two-dimensional solute transport and insignificant vertical density gradients, 4) conservative dispersed contaminant, and 5) groundwater extraction rates that are unchanging with time during the planning period (This requires fewer variables than would be needed if pumping varies with time. Subject to computer memory and optimization algorithm limitations, pumping rates can be permitted to vary with time.)

The purpose of the proposed model is to develop volumetrically optimal groundwater extraction strategies that assure acceptable future groundwater quality. We wish concentrations predicted by the optimization model to be as accurate as possible, but recognize that optimization models cannot generally use as fine a discretization in time or space as simulation models. Therefore, it is desirable to be able to improve the accuracy of the transport predicted by the optimization models. For this reason, the MODCON procedure includes calibration of optimization module solute transport equations with respect to solute transport predicted via a more detailed simulation module. Furthermore, simulation, calibration and optimization are performed cyclically until satisfactory similarity exists between concentrations predicted by optimization and simulation modules.

The MODCON procedure, outlined in Figure 1, consists of four optimization/simulation modules (A,B,D,E) and a simulation module (C). All modules are written using GAMS/MINOS (Kendrick and Meeraus, 1985; Murtagh and Saunders, 1983). Components A, B and E incorporate the two-dimensional linearized Boussinesq equation to model groundwater flow. Module C utilizes method of characteristics solute transport simulation. The function of module C can also be accomplished using an external simulation model.



1. Flowchart of module functions in MODCON.

(Konikow and Bredehoeft, 1978). Modules D and E incorporate implicit or explicit solute transport equations and linear influence coefficients. The functions of each part of MODCON are discussed below. Figure 2 illustrates the most important characteristics of each module.

The use of module A is optional. It performs steady-state flow simulation and weighted linear goal programming (LGP) optimization to determine acceptable boundary flux rates for the study area. This function is important when it is impractical to model an entire aquifer system. It aids developing a pumping strategy for only a portion of the aquifer (a subsystem) in such a way as to prevent disruption of flow outside that subsystem. To do this, an assumption that must be valid is that aquifer stimuli outside the system during the management period will maintain the regional flow patterns that exist at the beginning of the era (t=0), as long as pumping within the subsystem does not induce more groundwater flow into the subsystem than occurred initially. The recharge fluxes computed for boundary cells by module A can be used as upper limits on recharge in subsequent optimization modules.

As written, module B uses unsteady flow simulation and weighted LGP optimization to compute a pumping strategy that will

Module	Module Objective Type; Output	Constraints (c:) and bounds (b:)
A	Linear goal-programming (LGP) Optimization; Steady boundary fluxes $\{Q^*\}$ that best maintain initial heads.	c: 2D steady flow c: LGP for head b: on head
B	LGP Optimization; Pumping strategy $\{Q^*\}$ that best attains target subsystem heads $\{H^t_k\}$ by time k. Predicted heads $\{H^*\}$	c: 2D unsteady flow c: LGP for head b: on head b: on pumping
C	Nonlinear MOC solute transport Simulation; Future concentrations $\{C^C_k\}$ resulting from $\{Q^*\}$.	Simulation of: 2D unsteady flow 2D advect-dispersion
D	LGP Optimization; Calibrated coefficients $\{F^p\},\{F^r\},\{F^d\}$ so $\{C^D_k\}=\{C^C_k\}$	c: 2D advect-dispersion c: LGP for conc. b: on coefficients
E	LGP Optimization; Modified pumping strategy $\{Q^*\}$ that best attains target heads and achieves satisfactory concentrations $\{C^E_k\}$	c: 2D unsteady flow c: LGP for head c: 2D advect-dispersion c: LGP for conc. b: on head b: on pumping

Figure 2. Significant characteristics of MODCON modules

cause future potentiometric heads to be as close to target heads as possible. These target heads can be the heads that exist at t=0. They may also be the future desirable heads computed by other optimization models, such as models that maximize groundwater extraction or the economic benefit from groundwater use. Alternatively, the existing objective function of module B can be replaced with a function representing those goals directly.

Module C uses nonlinear solute transport simulation to compute future concentrations that will result from implementation of the pumping strategy computed by module B. If future concentrations will be unacceptable in some locations, the pumping strategy will need to be modified. To accomplish strategy modification, solute transport must be appropriately included in a model similar to module B. This is ultimately achieved in module E, after invoking module D.

Module D uses LGP to calibrate two-dimensional implicit or explicit solute transport equations so that they can replicate concentrations predicted by module C. When module D uses implicit equations, or explicit equations with more than one time step, its solute transport equations are nonlinear. The use of nonlinear constraints is acceptable when one is grateful simply to have a valid strategy and global optimality of the solution is

not critical.

Module E includes the objective function and unsteady volumetric simulation of module B, as well as the calibrated linear solute transport equations of module D. It develops a modified pumping strategy that considers groundwater quality constraints.

Because of the relatively coarse discretization used in module E, one should verify the concentrations predicted by that module. Module C, or an external simulation model, is used for that purpose. Figure 1 shows that iteration through modules D, E and C is continued until concentrations predicted by module E are acceptably close to those predicted by module C, or its substitute.

B. Model Development

For a n cell subsystem, the generic objective function for modules, A, B, D and E can be expressed as a variation of that shown by Yazdanian and Peralta (1986).

minimize y =

$$(W)\{D^{+}\} + (W)\{D^{-}\} + g\,(W^{+c})\{D^{+c}\} + g\,(W^{-c})\{D^{-c}\} \qquad ..[1]$$

where

(W) = a 1 x n vector of weighting factors for head,

(dimensionless)

$\{ D^{+} \}$ and $\{ D^{-} \}$ are n x 1 column vectors of nonegative over- and under-achievement variables for final heads, (L)

g = dummy factor to convert concentration into head, (L/ppm)

$\{ W^{+c} \}$ and $\{ W^{-c} \}$ are 1 x n vectors of weighting factors applied to those final concentrations that exceed or are less than target concentrations, respectively, (dimensionless)

$\{ D^{+c} \}$ and $\{ D^{-c} \}$ are n x 1 column vectors of nonegative over- and under-achievement variables for final concentrations, (ppm)

Modules A and B use only those portions of equation [1] that contain weights and achievement variables for head. Module D uses only weights and achievement variables for concentration. Module E uses the full equation and weights and achievement variables for both heads and concentrations.

Optimal solutions for modules A and B are constrained subject to the following, simply described for either steady-state flow (module A) or unsteady flow (module B). Equation [2] is a matrix representation of the implicit finite-difference two-

dimensional linearized flow equation. In the following equations, for k time steps, vectors of magnitude n become n x k.

$$\{ Q^{L} \} \leq \{ Q^{*} \} = \{ B \} - [A] \{ H^{*} \} \leq \{ Q^{U} \} \quad ..[2]$$

$$\{ H^{L} \} \leq \{ H^{*} \} \leq \{ H^{U} \} \quad ..[3]$$

$$\{ H^{*} \} - \{ D^{+} \} + \{ D^{-} \} = \{ H^{t} \} \quad ..[4]$$

$$0.0 \leq \{ D^{+} \}, \{ D^{-} \} \quad ..[5]$$

where

$\{ Q^{L} \}$ and $\{ Q^{U} \}$ = n x 1 column vectors of lower and upper bounds, respectively, on pumping (or recharge), (L^3T^{-1})

$\{ Q^{*} \}$ = n x 1 column vector of optimal net steady pumping (or recharge) rates, where discharge is positive-valued, (L^3T^{-1})

$\{ B \}$ = n x 1 vector describing the change in storage with time, (L^3T^{-1}). $\{ B \}$ is a zero vector for steady-state flow.

$[A]$ = n x n symmetric banded matrix of aquifer properties, (L^2T^{-1})

$\{ H^{*} \}$ = n x 1 column vector of optimal final or intermediate heads, depending on the number of time steps, (L)

$\{ H^L \}$ and $\{ H^U \}$ = n x 1 column vectors of lower and upper bounds on head, (L)

$\{ H^t \}$ = target heads, (L)

Note that the objective function considers all cells, not merely internal cells. In this example, through equations [2,3], boundary cells are treated as variable head/restrained flux boundary conditions, rather than as classical constant head (Dirichlet) or constant flux (Neumann). The use of weights of large magnitude for boundary cells effectively forces heads to closely approximate desired values.

Module C is a simulation model of two-dimensional advection and dispersion of a conservative contaminant. It performs no optimization. It is a GAMS representation of the FORTRAN method of characteristics code developed by Konikow and Bredehoeft (1978). Here five particles are used initially in each cell.

As previously stated, the function of module D is to calibrate implicit or explicit finite difference advective solute transport equations so that they will predict the same concentrations as the potentially more accurate module C. The change in concentration due to dispersion as computed by module C is used directly in modules D and E. Thus neither D nor E need to include the nonlinear dispersion equations. The MODCON iteration

procedure serves to cause convergence between the change in concentration caused by dispersion assumed in modules D and E, and the values computed by module C.

Module D uses the latter half of objective function [1] subject to constraints and bounds [6-9] mentioned below. The objective function of module D usually applies the same weight to both over- or under-achievement variables for concentration. In practical application it has been useful to also include in the objective function the sum of all f^r and f^d coefficients (defined below). These are included to make their values be as small as practical. This forces them to be zero when no contaminant needs to be moved between cells. To maintain consistency in units while implementing this artifice, these coeficients must be multiplied by one linear unit.

In subsequent discussion, variables or constants used to describe values for individual cells are shown using lower-case letters, as opposed to the upper-case notation used for vectors. For brevity, definitions of lower-case terms are omitted if definitions have already been provided for analagous vectors.

$$\{ C_k^D \} - \{ D^{+c} \} + \{ D^{-c} \} = \{ C_k^C \} \qquad ..[6]$$

$$0.0 \leq \{ D^{+c} \}, \{ D^{-c} \} \qquad ..[7]$$

$$0.0 \leq \{ F^{p} \} \leq \{ F^{pU} \} \quad ..[8]$$

$$0.0 \leq \{ F^{r} \}, \{ F^{d} \} \leq \{ F^{rU} \} \quad ..[9]$$

where

$\{ C_k^D \}$ and $\{ C_k^C \}$ are n x 1 vectors of the concentrations predicted for the end of the final time time step, using modules D and C, respectively, (ppm)

$\{ F^{p} \}$, $\{ F^{r} \}$ and $\{ F^{d} \}$ are n x 1 vectors of coefficients being applied to solute transport due to pumping in a cell and due to advection across the right-hand face and the down-side face of that cell respectively (dimensionless)

$\{ F^{pU} \}$ and $\{ F^{rU} \}$ are upper bounds on the coefficients applied to solute movement either due to extraction by pumping, or due to advection, (dimensionless)

Within module D, concentration at a cell located in row i and column j at the end of time step k is computed using the grid system shown in Figure 3. For a cell (i,j), midpoint terms with d superscripts (f, t and v) apply to the boundary between cell

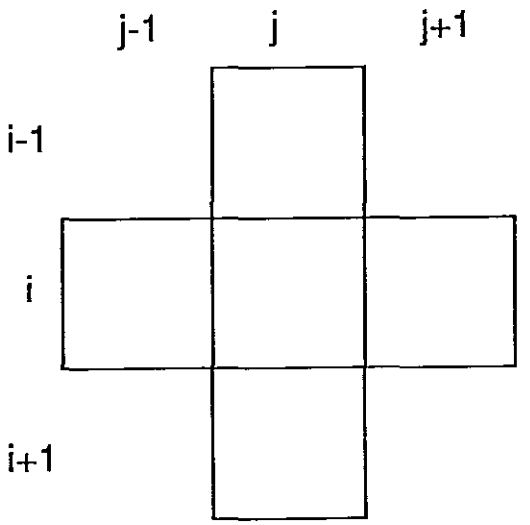


Figure 3. Cell grid notation system for finite difference equations.

(i,j) and cell (i+1,j). Midpoint terms with r superscripts apply to the boundary between cell (i,j) and cell (i,j+1). Because the same f coefficients apply to cells on both sides of a boundary, mass balance is maintained. The same amount of contaminant leaves through a boundary as enters the cell on the other side of the boundary.

Equation 10 is the implicit finite-difference equation that is used for advective solute transport. (It can be converted into an explicit form by using c_{k-1} to compute the t terms in Equations [11-15].) For all active cells i,j in the subsystem:

$$c_{i,j,k} = c_{i,j,k-1}\left(1 - f^{p}_{i,j}\frac{q_{i,j,k}\,\Delta t}{S\,T_{i,j}\,\Delta x^{2}}\right) + d_{i,j,k}$$

$$- f^{r}_{i,j}\,t^{r}_{i,j,k} + f^{r}_{i,j-1}\,t^{r}_{i,j-1,k} - f^{d}_{i,j}\,t^{d}_{i,j,k} + f^{d}_{i-1,j}\,t^{d}_{i-1,j,k} \qquad ..[10]$$

where

$q_{i,j,k}$ = pumping or recharge in cell i,j, time step k, (L^3T^{-1})

Δt = length of time step, (T)

S = effective porosity, (dimensionless)

$T_{i,j}$ = saturated thickness in cell i,j, (L)

Δx = length of a cell side, (L)

$d^{k}_{i,j,k}$ = change in concentration in cell i,j due to dispersion, as computed by module C, based on the concentrations existing at the beginning of time step k, (ppm)

$t^{r}_{i,j}$ and $t^{d}_{i,j}$ = change in concentration in cell i,j caused by advection across a cell boundary, (ppm)

$$t^{r}_{i,j,k} = -\frac{\Delta t}{\Delta x} v_{i,j,k} c_{i,j+1/2,k} \quad ..[11]$$

$$t^{r}_{i,j-1,k} = \frac{\Delta t}{\Delta x} v_{i,j-1,k} c_{i,j-1/2,k} \quad ..[12]$$

$$t^{d}_{i,j,k} = -\frac{\Delta t}{\Delta x} v_{i,j,k} c_{i+1/2,j,k} \quad ..[13]$$

$$t^{d}_{i-1,j,k} = \frac{\Delta t}{\Delta x} v_{i-1,j,k} c_{i-1/2,j,k} \quad ..[14]$$

$$v^{r}_{i,j,k} = \frac{K}{S} (h_{i,j,k} - h_{i,j+1,k}) \quad ..[15]$$

= velocity of solute movement between cell i,j and cell i,j+1, (L/T). Since v^{r} denotes 'to the right', v^{d} denotes 'down' in a plan view.

$$c_{i,j+1/2,k} = \frac{c_{i,j,k} + c_{i,j+1,k}}{2} \quad ..[16]$$

= midpoint concentration between cell i,j and cell i,j+1, (ppm)

Expressions analagous to equation [15] exist for the other three velocities shown in equations [12-14]. Similarly, there are equations analagous to [16] for the other three midpoint concentrations shown in equations [12-14].

In module D, heads used to compute velocities in equations [11-14] are known for all time steps, having been computed earlier in module B. The concentrations used in equations [11-14] are unknown variables. The f coefficients are also variables whose values are optimized in the module. Thus, implicit advective transport equations are nonlinear. An explicit transport formulation is linear for a single time step, but is nonlinear for multiple time steps.

Module E utilizes objective function [1], constraint equations [2-5] for unsteady flow simulation and equations [7-9,17] for solute transport simulation.

$$\{ C^{E}_{k} \} - \{ D^{+c} \} + \{ D^{-c} \} = \{ C^{t}_{k} \} \quad ..[17]$$

where

$\{ C^{E}_{k} \}$ = a n x 1 vector of the final concentrations resulting at the end of time step k from optimal pumping in module E, (ppm)

$\{ C^{t}_{k} \}$ = a n x 1 vector of target concentrations, i.e. the upper limit on acceptable concentrations resulting at the end of the planning period, (ppm). These target concentrations are predetermined by management agency.

Equation [17] is a 'soft' constraint in that it is possible to exceed the final concentrations. In practice, using a large W^{+c} and relatively small values of W^{-c} and W in the objective function causes target concentrations to be attained if it is physically feasible to do so.

In Module E, pumping values and future concentrations and heads are unknown variables. Even though the f coefficients are known from Module D, transport constraints are nonlinear. Dispersion is still treated as a known value, having last been computed in module C. The error in the assumed transport due to dispersion is corrected through the process of iterating through modules C, D and E.

An alternative to using the five-module MODCON approach is to use Module E by itself. In that case, all f coefficients have values of 1.0 and implicit or explicit solute transport simulation is used. A Crank-Nicolson formulation might also be used. That approach is practical if one can accept the error caused by crude discretization. It permits one to forego the process of iterating through modules C, D and E. In that case, Module A would probably be used only to determine limits on boundary recharge rates.

PRINCIPAL FINDINGS AND SIGNIFICANCE

A. Testing of Explicit Solute Transport Form of MODCON

A hypothetical unstressed steady-state system is assumed (Figure 4). Flow assumptions are as mentioned previously. An effective porosity of 0.3 and a transmissivity of 1,092 m^2/day (11,750 ft^2/day) are assumed. In this test contaminant movement occurs only by advection (dispersivity equals zero).

Effective weights of 1 are assumed for head over- and under-achievement variables in modules A, B and E. Weights of 1 are used for concentration over- and under-achievement variables in module D. In module E weights of 1,000 and 1 are used for concentration over- and under-achievement variables respectively. Thus module E attempts to insure that concentrations do not exceed target concentrations. If necessary, the same emphasis can be achieved in module D by increasing the magnitude of the achievement variables for concentration. All f coefficients are bounded to be between 0.0 and 10.0 in value.

Lower bounds on recharge and discharge are zero. Upper bounds are a large enough value that they never are restrictive. All constant-head cells are permitted to either discharge or accept recharge, depending on what the model prefers. Discharge is also permitted at all internal cells, but recharge can occur only at cells (9,4), (9,5) and (9,6). Potentiometric heads

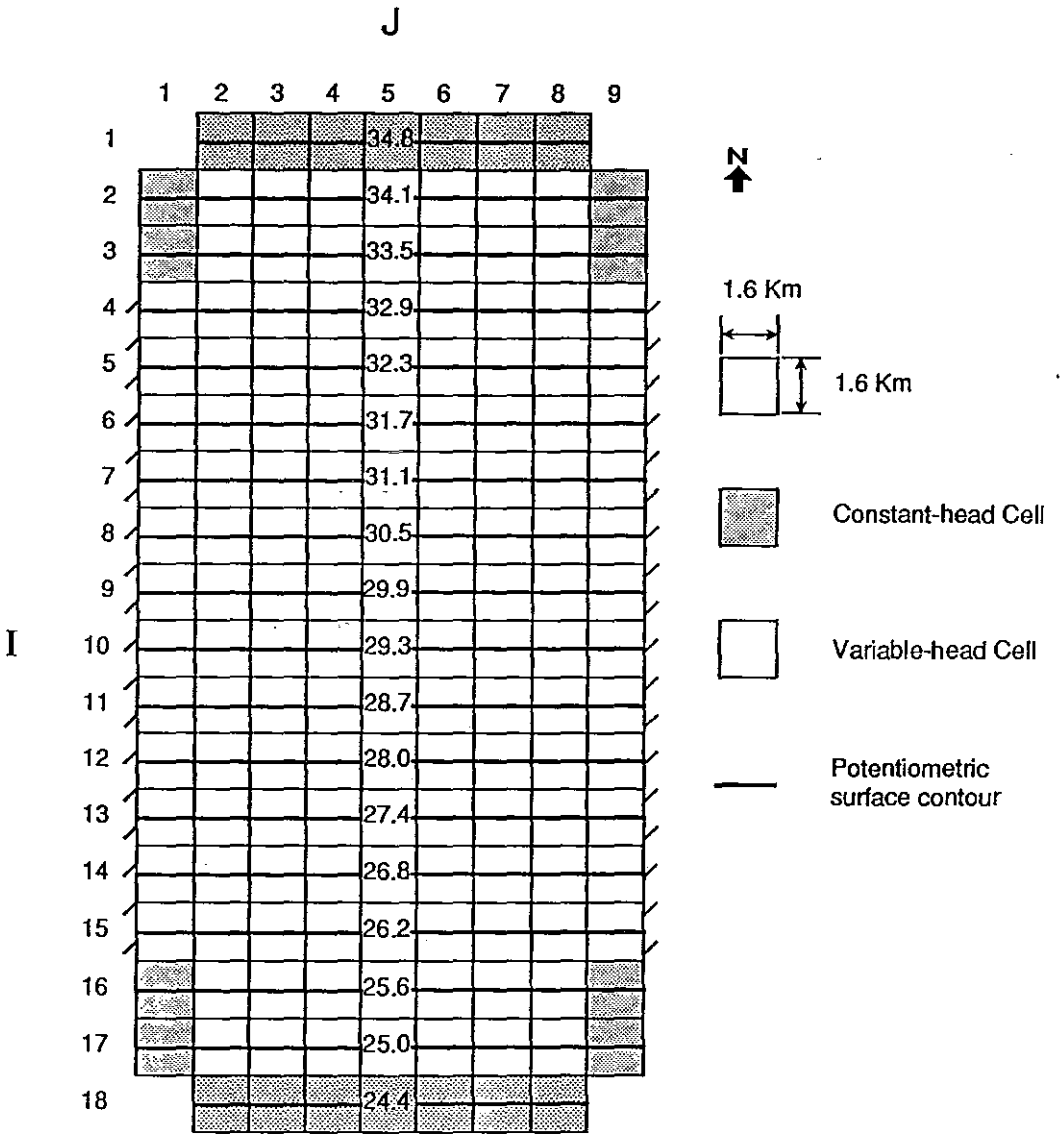


Figure 4. Assumed initial potentiometric surface in hypothetical study area, in m above sea level.

can change as long as they do not exceed the ground surface elevation. They never approach that limit in tested situations.

Figure 5 shows the initial salinity concentrations that are assumed. Figure 6 shows the concentrations that will result after 25 years of steady-state flow, assuming no addition of contaminant to the system. Values shown in Figure 6 are computed using two 12.5-year time steps. Concentrations predicted using twenty-five one-year time steps or a single 25-year step are within 10 ppm of the displayed values. Accordingly, MODCON modules discussed below use two 12.5 year time steps. To reduce computational requirements, optimal pumping is steady in time. Head response to pumping is transient.

Assume that a management agency wishes to assure that 25-year concentrations in target cells (9,5), (9,6) and (9,7) do not exceed 200 ppm. In Figures 5 and 6 we see that initial concentrations in those cells are 375 ppm and 25-year concentrations without management are 390 ppm. Clearly some extraction or injection of water to the aquifer is needed to achieve the management objective.

In the initial iteration of the MODCON modules, the explicit form of module E computes the optimal pumping values shown in Figure 7a. Note that total discharge and recharge rates via wells are 927 and 917 10^3 m^3yr^{-1} (751 and 743 ac-ft yr^{-1}) respectively.

I \ J	1	2	3	4	5	6	7	8	9
1		0	0	0	0	0	0	0	
2	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0
5	0	0	550	550	550	550	550	0	0
6	0	0	550	550	550	550	550	0	0
7	0	0	450	450	450	450	450	0	0
8	0	0	400	400	400	400	400	0	0
9	0	0	380	375	375	375	380	0	0
10	0	0	350	350	350	350	350	0	0
11	0	0	325	325	325	325	325	0	0
12	0	0	300	300	300	300	300	0	0
13	0	0	270	270	270	270	270	0	0
14	0	0	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	0	0
18		0	0	0	0	0	0	0	

Figure 5. Assumed initial NaCl concentrations in groundwater, in ppm.

		J							
	1	2	3	4	5	6	7	8	9
1		0	0	0	0	0	0	0	
2	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0
5	0	0	220	220	220	220	220	0	0
6	0	0	530	530	530	530	530	0	0
7	0	0	480	480	480	480	480	0	0
8	0	0	430	430	430	430	430	0	0
9	0	0	392	390	390	390	392	0	0
10	0	0	368	365	365	365	368	0	0
11	0	0	340	340	340	340	340	0	0
12	0	0	315	315	315	315	315	0	0
13	0	0	288	288	288	288	288	0	0
14	0	0	162	162	162	162	162	0	0
15	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0	0	0
18		0	0	0	0	0	0	0	

I

Figure 6. Concentrations that will result after 25 years without pumping, in ppm.

a)

I \ J	2	3	4	5	6	7	8
7	0	0	0	0	0	0	0
8	0	0	15	59	15	0	0
9	0	27	[-94	-22	-94]	27	0
10	0	0	15	58	15	0	0
11	0	0	0	0	0	0	0

b)

I \ J	2	3	4	5	6	7	8
7	0	0	0	0	0	0	0
8	0	0	20	71	20	0	0
9	0	33	[-112	-62	-112]	33	0
10	0	0	18	75	78	0	0
11	0	0	0	0	0	0	0

Figure 7. Optimal groundwater extraction (+) and injection (-) rates computed by two versions of module E in $10^3 m^3/yr$:
a) explicit form of solute transport equation,
b) implicit solute transport equation.

Since the model attempts to disrupt regional heads as little as possible, total discharge and recharge rates are very similar in magnitude.

Module E also predicts that as a result of that pumping, concentrations of precisely 200 ppm will be attained by year 25 in the target cells. Subsequent reuse of module C shows the concentrations that would more probably occur (Figure 8). Note concentrations of 195, 205 and 195 in cells (9,4), (9,5) and (9,6) respectively. Assuming that a concentration of 205 ppm is close enough to 200 to be acceptable, the flow chart of Figure 2 indicates that no more iterations are necessary.

For demonstration purposes however, modules D, E and C are run again and provide the following results. After recalibrating the f coefficients in module D to emulate the concentrations projected by the second use of module C, module E computes a new pumping strategy. Again module E expects this strategy to cause 200 ppm concentrations in the three target cells. In the new strategy total discharge and recharge by wells is 965 and 967 10^3 m^3 yr^{-1} (782 and 783 ac-ft yr^{-1}) respectively. These represent 4 to 5 percent increases from the results of the previous iteration.

According to the module C MOC model, concentrations that would result from implementing the revised pumping strategy are 191, 219 and 202 ppm for cells (9,4), (9,5) and (9,6). For these target cells, this

		J							
		1	2	3	4	5	6	7	8	9
I	1	0	0	0	0	0	0	0	0	0
	2	0	0	0	0	0	0	0	0	0
	3	0	0	0	0	0	0	0	0	0
	4	0	0	0	0	0	0	0	0	0
	5	0	0	220	220	220	220	220	0	0
	6	0	0	530	530	530	530	530	0	0
	7	0	0	480	480	480	480	480	0	0
	8	0	0	430	425	425	425	430	0	0
	9	0	0	392	195	205	195	392	0	0
	10	0	0	368	299	337	299	368	0	0
	11	0	0	340	340	340	340	340	0	0
	12	0	0	315	315	315	315	315	0	0
	13	0	0	288	288	288	288	288	0	0
	14	0	0	162	162	162	162	162	0	0
	15	0	0	0	0	0	0	0	0	0
	16	0	0	0	0	0	0	0	0	0
	17	0	0	0	0	0	0	0	0	0
	18	0	0	0	0	0	0	0	0	0

Figure 8. Concentrations that will result after 25 years of pumping at optimal rates computed by explicit version of module E, in ppm.

result is less accurate than that predicted in the first iteration.

When all contaminated cells are considered however, iteration seems to improve the overall accuracy of the presented linear coefficient simulation scheme. The sum of the absolute values of all differences between future concentrations predicted by first iteration use of the explicit module E and subsequent use of MOC simulation is 600 ppm (average of 12 ppm per contaminated cell). On the other hand the sum of all positive and negative-valued differences in concentration computed by E and C, (E - C) is only 24 ppm. Analagous sum of absolute-valued differences computed using the second iteration results from module E is 535 (average of 11 ppm per contaminated cell). In this case the sum of concentration differences between E and C is - 57 ppm.

As long as there is difference between the heads used to calibrate module D and the heads computed by subsequent optimization in module E, one expects some error in concentrations predicted by module E. After all, modules D and E use explicit or implicit representations of the partial differential expression of solute transport, while module C uses a method of characteristics particle tracking method.

The f coefficients in modules D and E permit advective transport to be increased or decreased to match that predicted by MOC simulation (or any other sort of prediction used in module C). For example in modules D and E, unless the f coefficient describing advective

transport equals zero, if there is contaminant in a cell, some of that contaminant will move to an adjacent cell if water flows to that cell from the contaminated cell. On the other hand, in a MOC model, contaminant will appear in the down-gradient cell only if characteristic particles travel far enough to cross the cell boundary. If particles do not traverse cell boundaries, then a MOC model will predict no concentration in the down-gradient cell. Through use of coefficients, modules D and E can match MOC-predicted concentrations.

The tested scenario provides a more rigorous test of the model than would be imposed if there is originally no contamination in the target cells and if no contaminant should enter them. In that case, the model merely needs to pump in such a way as to prevent migration due to advection. This can be accomplished by causing heads in the target cells to be greater than those in surrounding cells. That simple approach is commonly used in management models that do not incorporate solute transport equations.

The simple hydraulic gradient control approach is inadequate if some contaminant is acceptable in target cells and if contaminant initially exists in those cells. In this case, the MODCON procedure ensures that final concentration is acceptable. It causes the development of hydraulic gradients that simultaneously limit the inflow of contaminant while flushing existing contaminant out of the target cells. Figure 9 shows the changes in potentiometric surface elevations

I

J	2	3	4	5	6	7	8
5	.0	.0	-.01	-.01	-.01	.0	.0
6	.0	.0	-.01	-.01	-.01	-.01	.0
7	.0	.0	-.01	-.04	-.01	.0	.0
8	.0	.0	-.01	-.10	-.01	.0	.0
9	.0	.01	[.27	.17	.27]	.01	.0
10	.0	.0	.01	-.10	.01	.0	.0
11	.0	.0	.01	-.03	.0	.0	.0
12	.0	-.01	-.01	-.02	-.01	-.01	.0
13	.0	-.01	-.01	-.01	-.01	.0	.0

Figure 9. Change in potentiometric surface elevation by year 25 caused by optimal pumping computed in first iteration using explicit version of module E, in meters.

that result from the optimal extraction and injection strategy. Figure 10 shows that although the gradient is changed it is not reversed to the extent that contaminant from up-gradient no longer enters the target cells.

The MODCON strategy slows contaminant entry to the target cells and hastens contaminant exit. This is seen by observing head differences between cells immediately above and below the target cells. Note that initially there is a uniform 2-foot drop in head per mile (per row). By year 25, the drop between rows 8 and 9 for columns 4, 5 and 6 has decreased to 1.123, 1.088 and 1.123 feet respectively. These correspond to gradient and contaminant velocity decreases of 44, 46 and 44 percent respectively. By the same time the head drop between rows 9 and 10 has increased to 2.877, 2.9 and 2.877 feet, corresponding to velocity increases of 43, 45 and 43 percent respectively.

Although the presented methodology seems to adequately achieve desired concentrations, one may question whether computed strategies are optimal from other perspectives. In this example, one part of the objective function of module E attempts to maintain initial heads to the extent possible. Thus, that function includes the sum of differences between 25 year heads resulting from the optimal strategy and those heads that would result from no pumping. It also contains the weighted concentration achievement variables. For this

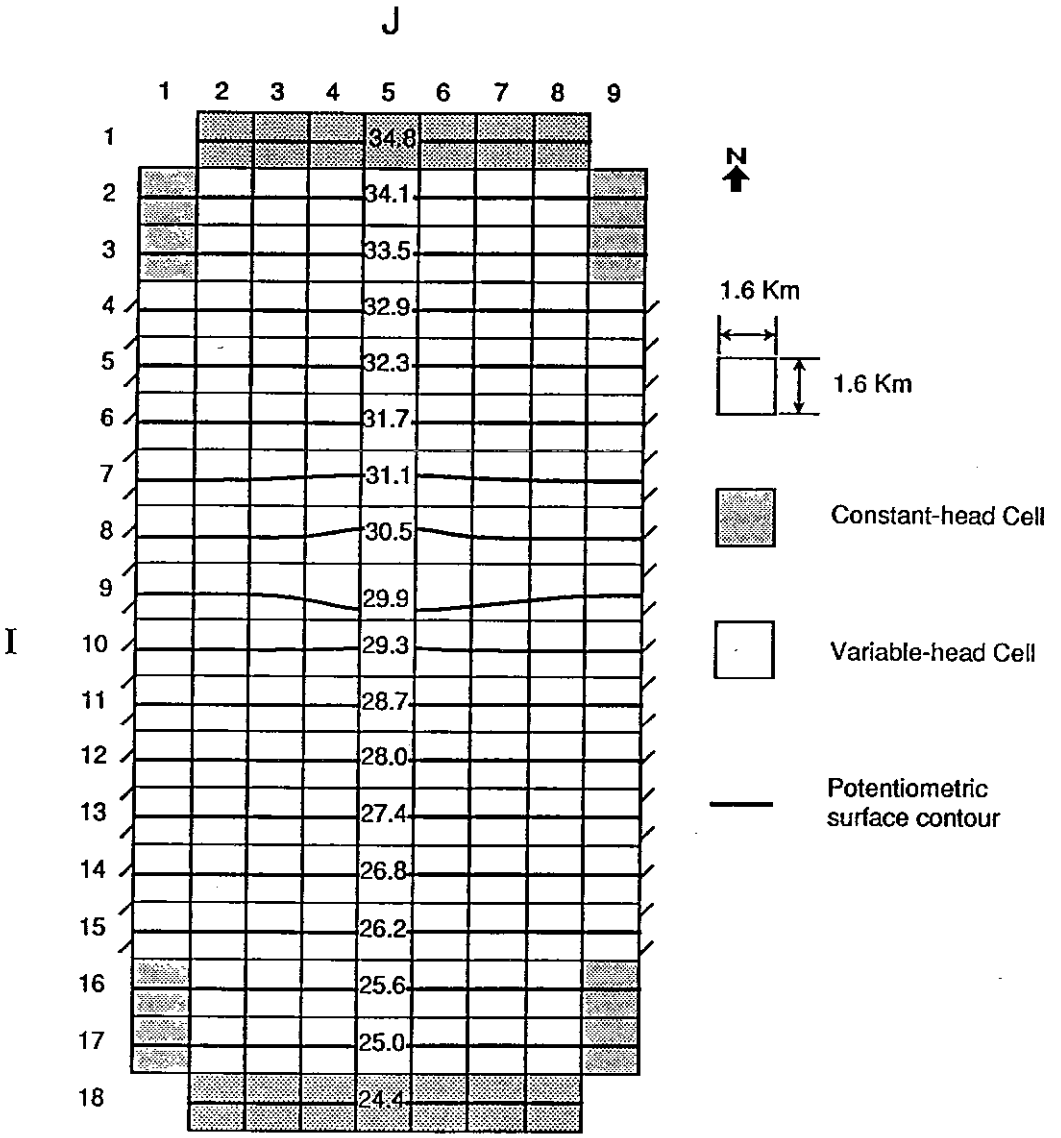


Figure 10. Heads that will result after 25 years of pumping at optimal rates computed by explicit version of module E, in m above sea level.

multiobjective problem, weights are used to emphasize one objective versus another. When objectives are in conflict optimal strategies lie on the pareto optimum and enhancing attainment of one objective can only be accomplished by harming attainment of the other. In such a case it is common practice to compute trade-off functions for selected strategies. These describe the change in one objective caused by an incremental change in the other objective.

There is a particular advantage to using head achievement variables in the objective function. As mentioned previously, the target heads may be those developed by a 'target design' management model before invoking MODCON. They may be steady-state heads or transient heads computed as being optimal for the end of the planning period. They may be developed by models with objective functions that maximize economic or other benefits. By seeking to maintain those heads to the extent possible, module E seeks to disrupt the previously developed optimal strategies as little as possible, while satisfying qualitative goals. A simple example of this decomposition process occurs if the preliminary optimization model computes a pumping strategy that maximizes volumetric extraction of groundwater. Associated with that strategy are the heads that will result at the end of the planning period. By using those heads as its 'target' heads, MODCON seeks to disrupt the volumetrically optimal strategy as little as possible, while achieving target concentrations.

One may ask why recharge should be used and target concentrations should not be achieved using only extraction. If only discharge wells are used, there is a much greater disruption of the regional flow than if both discharge and recharge are used. This somewhat negates the benefits of using the target head achievement component of the objective function of module E. Furthermore, when using internal discharge but no recharge, concentrations predicted by module E in a preliminary iteration are much less accurate than those presented and discussed above. In this case Module C demonstrates that implementing the optimal extraction strategy results in concentrations of about 300 ppm in the target cells. This occurs because as the differences in head between those assumed by modules C and D and those computed by E increase, predictive error also increases.

Justification for using recharge only at target cells is found by performing preliminary optimizations using MODCON. If left free to recharge or discharge at all internal cells, module E computes total discharge and recharge of 1,175 and 1,218 10^3 m^3 yr^{-1} (952 and 987 ac-ft yr^{-1}). Although most of the recharge occurs at the target cells, some occurs up to two rows away. Since the objective function does not attempt to minimize total pumping, the model does not of itself consider the practical aspects of having to recharge at many different locations. For management purposes, concentrating recharge at target cells is most reasonable. In addition, total pumping is less when

concentrated.

B. Comparison of Explicit and Implicit Solute Transport Versions of MODCON

For the problem described above, optimal annual pumping computed by an implicit solute-transport version of MODCON is shown in Figure 7b. Discharge and recharge through wells each total about 1,160 10^3 m^3 yr^{-1} (940 and 938 ac-ft yr^{-1} respectively). These rates are about 125 percent of the respective pumping rates computed by the explicit model.

Above we describe error as the sum of the absolute-valued or real differences between concentrations predicted by modules E and C. Total absolute valued error of the implicit model is 125 percent of that of the explicit model (750 versus 600 ppm). Total real-valued error is almost ten times that of the explicit model (-250 versus +24 ppm). In addition, error in concentrations computed for the target cells in the first iteration is slightly greater for the implicit than the explicit version. Module C projected concentrations of 205, 211 and 205 ppm in cells (9,4), (9,5) and (9,6) respectively, when using the optimal strategy from the implicit model. Since the implicit module E predicted concentrations of 200 ppm in all three cells, it underestimated by a total of 21 ppm. The explicit module E on the other hand overestimated by a total of 5 ppm. In the described scenario, a manager would generally prefer that his model overestimate

future concentrations, rather than underestimate them.

In the performed comparison, coefficients computed by the explicit module D predict future concentrations better than those computed by an implicit module--at least when heads and pumping values change from those assumed in module D. For the explicit approach, values of f^p and f^r computed by module D are 1.0 and 0.0 respectively. For this approach f^d is either 0.0 (for cells without initial contamination) or between 1.113 and 1.890 (average of 1.226). For the implicit approach the values are 1.0, 0.0 and either 0.0 or between 1.095 and 1.467 (average of 1.181) respectively. One expects the implicit coefficients to be slightly smaller than the explicit coefficients because the implicit equations utilize concentrations at the end of each time step to predict advective transport, while the explicit equations utilize concentrations at the beginning of each time step. Because of the flow field, concentrations are increasing in more rows than they are decreasing (eight out of ten rows that have contaminated cells by year 25). Therefore there is slightly less need for coefficients in the implicit model to increase transport.

It is also useful to compare explicit and implicit models when including dispersion in MODCON. Assuming longitudinal and transverse dispersivities of 200 ft, both models were run for the same problem initially posed. The explicit model computed total discharge and recharge by wells as 884 and 923 10^3 m^3 yr^{-1} (716 and 748 ac-ft yr^{-1})

respectively. This slight decrease from pumping rates computed previously possibly results because the contaminant moves a little farther in the same time period even if gradients are unchanged. The implicit model pumps about the same as previously, discharging 1,167 10^3 m^3 yr^{-1} (945 ac-ft yr^{-1}) and recharging 1,160 10^3 m^3 yr^{-1} (940 ac-ft yr^{-1}).

The accuracy of concentrations predicted by explicit and implicit models using dispersion are similar. Both versions of module E predicted concentrations of 200 ppm in the three target cells. When testing the optimal strategy computed by the explicit model, module C predicted concentrations of 207, 209 and 207 ppm from left to right in those cells. When testing the strategy developed by implicit model, module C predicted concentrations of 207, 212 and 207 ppm.

For unexplained reasons, neither explicit nor implicit versions of Module E can compute optimal solutions if all f coefficients are assigned values of 1.0. This precludes the use of an uncalibrated Module E and means that it functioned satisfactorily only when used as part of the MODCON procedure.

The explicit form of MODCON requires less computer processing time than does the implicit version. In this report, all processing is accomplished using an IBM 4381 mainframe computer running under VM/CMS. Average CPU time required to run all five modules in the explicit version for the above problem is 91.5 minutes. The implicit

version required about 127 minutes, 139 percent of the explicit requirement. Assuming that the module D calibration process eliminates the possibility of numerical instability in the explicit approach, the explicit version of MODCON seems preferable to the implicit version.

CONCLUSIONS

A methodology for simulating conservative solute transport within computer models for optimizing groundwater management is presented. The technique allows the achievement of 'target' groundwater contaminant concentrations within groundwater use strategies that may optimize attainment of volumetric, economic or other policy objectives. The technique differs from the more common approach of preventing contaminant migration by absolutely restricting advective movement. The presented method is flexible in that advective contaminant movement may be permitted toward and through concentration control cells. This is especially valuable if some contamination already exists within a control cell, or if preventing contaminant movement through such cells may be economically or technically impractical.

The technique utilizes a five module approach consisting of four optimization modules and a single simulation module. The first two modules optimize volumetric management and do not consider groundwater quality constraints. They utilize the embedding approach for representing steady or transient groundwater flow. The third module

simulates advective/dispersive solute transport using the method of characteristics. It performs no optimization. The fourth module uses optimization to compute linear coefficients that best calibrate explicit or implicit transport difference equations. The fifth module combines unsteady flow and calibrated solute transport equations to develop a volumetric strategy that achieves target concentrations as much as possible.

Comparisons performed for a hypothetical system show that an explicit form of calibrated solute transport equation requires significantly less computer processing time than an implicit formulation. In addition, probably because of the calibration process, the explicit form yields answers that are at least as accurate as those from an implicit representation.

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