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Optimizing perennial groundwater yield planning for nonlinear systems: approach comparison

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OPTIMIZING PERENNIAL GROUNDWATER YIELD
PLANNING FOR NONLINEAR SYSTEMS:
APPROACH COMPARISON

by Shu Takahashi &
Richard C. Peralta

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OPTIMIZING PERENNIAL GROUNDWATER YIELD PLANNING FOR NONLINEAR SYSTEMS: APPROACH COMPARISON

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OPTIMIZING PERENNIAL GROUNDWATER YIELD PLANNING FOR NONLINEAR SYSTEMS: APPROACH COMPARISON

by Shu Takahashi and Richard C. Peralta

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Abstract

Four alternative simulation/optimization models useful for computing optimal sustained-yield (steady-state) groundwater pumping strategies are compared in terms of formulation, solution procedure, accuracy, and computational efficiency. The different models require different computer processing time and memory. For the aquifer tested system, if more than 10% of the cells have pumping as a decision variable, a fully linearized embedding model will require less computer memory than any other model. All the models address linear and nonlinear steady-state flow in multilayer, unconfined/confined aquifers. They also address several types of nonsmooth external flows. Newly presented are a response matrix model solving external flows described by nonsmooth functions through cycling, and a fully nonlinear embedding model that directly achieves an optimal solution without cycling. Models are tested using a hypothetical three-layer (unconfined/confined) aquifer system (3 layers x 15 rows x 15 columns = 675 cells). Empirically, globally optimal solutions seem to be obtained. All the models compute the same optimal pumping even if their optimizations are begun using vastly different initial guesses. This addresses a common concern that the solutions to nonlinear problems are not necessarily globally optimal.
Introduction

Some groundwater management models can determine the best pumping strategy for a desired goal while simulating the aquifer response to that pumping. Such models generally use either the embedding or response matrix approach (Gorelick, 1983). Most models reported in the literature have been applied to linear systems or have assumed linearity. However, flow in many aquifers is nonlinear.

Numerical approximations of the saturated groundwater flow equation are either linear or nonlinear (for confined or unconfined, respectively). However, flows such as evapotranspiration, drain discharge, stream-aquifer interflow, and discharge from flowing (artesian) wells can be represented by nonsmooth functions which are not continuously differentiable. For such nonlinear flow systems, it is sometimes inappropriate to assume system linearity. Furthermore, it is sometimes not theoretically possible to prove that a solution is globally optimal.

The embedding approach directly incorporates numerical approximations of the groundwater flow equation in the model as constraints. It provides optimal solutions of head, pumping rate, and other variables at all cells simultaneously for the entire area. The feasibility of the embedding approach for groundwater management using the finite-difference approximation was tested by Aguado and Remson (1974). Both steady and unsteady conditions were considered for one-dimensional confined and unconfined aquifers. A
steady-state, two-dimensional confined aquifer example (15 cells) was also presented in the study.

Some researchers have summarized or reported computational difficulties of optimization algorithms for embedding models especially for transient problems (Gorelick, 1983; Tung and Kolterman, 1985; Yazdanian and Peralta, 1986). Others have successfully used the embedding approach for large and/or complex aquifer systems (Cantiller et al., 1988; Gharbi et al., 1990; Peralta et al., 1991a). The MINOS software (Murtagh and Saunders, 1987) was used to perform the optimization in the latter models.

The USU groundwater management model, USUGWM (Gharbi, 1991), is the first embedding model optimally managing a large, multilayer, and nonlinear aquifer system under transient conditions. Gharbi applied it to the Salt Lake Valley aquifer, which is discretized into 1,086 cells. Constraints describing flow in the unconfined aquifer, contaminant transport, stream-aquifer interflow, and evapotranspiration are formulated both linearly and nonlinearly. The model was cyclically solved to reach the optimal solution of the original nonlinear flow system. USUGWM overcame previously reported disadvantages of the embedding approach. It used nonlinear formulations of nonsmooth flow functions. However, USUGWM also used a linear surrogate to address the nonlinear transmissivity of an unconfined layer.
Recently, a differential dynamic programming (DDP) algorithm has been used for groundwater management (Jones et al., 1987; Culver and Shoemaker, 1992). Because of its decomposition, DDP overcomes the dimensionality problems associated with the embedding approach under transient conditions.

The response matrix approach relies on the principle of superposition to simulate groundwater flow. Influence coefficients describing potentiometric head response to unit pumping are first generated for specified locations using an external groundwater flow simulation model. A response matrix consisting of these influence coefficients is then used with superposition to compute heads in the management model. Because only influence coefficients for control locations are included, memory required by the response matrix optimization model can be minimized.

There have been many transient simulation or management models using the response matrix approach for various objectives. Among these models, Illangasekare and Morel-Seytoux (1982) presented a stream/aquifer simulation model using discrete kernels (influence coefficients). They (1984) also developed "reinitialization" and "scanning subsystem" techniques for creating and handling discrete kernels. These techniques can save computer storage to simulate in two dimensions the physical behavior of the large aquifer. These types of discrete kernels can be coupled with optimization problems.
Peralta and Kowalski (1986) used discrete kernels to determine optimal groundwater extraction strategies for the Grand Prairie of Arkansas. Peralta et al. (1988a) used resolvent influence coefficients for maximizing crop production in a hypothetical stream/aquifer system. These stream-stage and groundwater levels changed dynamically in response to pumping and inflow. Peralta et al. (1988b) used the response matrix approach to develop optimal groundwater extraction strategies including recharge basins for the study area. In that study, they used resolvent influence coefficients which expressed groundwater-level response to pumping and simultaneous interflow between a recharge basin and aquifer. Peralta et al. (1991) combined embedding, cell and well influence coefficients and superposition, with the stream-flow routine to represent dynamic stream stage and groundwater level interaction while optimizing conjunctive use.

Reichard (1987) used two types of influence coefficients, water level responses to a unit discharge and recharge, in the groundwater management model for the Salinas Valley of California. To address surface water-groundwater interaction, a river recharge function is embedded in the model.

Since superposition is most properly applicable to linear systems, assumptions or methods are required to apply it to nonlinear (unconfined) aquifers. Maddock (1974) developed a nonlinear, technological function for a one-dimensional unconfined aquifer system. Drawdown response to pumping is
represented by an infinite power series. A nonlinear, technological function is computed using a finite sum of the power series. The number of terms needed to achieve a good approximation was determined by the ratio of drawdown to saturated thickness. When this nonlinear, technological function is used in an optimization model, the objective function becomes a nonlinear formula.

Heidari (1982) applied the normal response matrix approach to groundwater management in the Pawnee Valley of southcentral Kansas. A one-layer, unconfined aquifer system was approximated as a confined aquifer, and the drawdown correction for the unconfined aquifer was calculated using the approach of Jacob (1944).

Danskin and Gorelick (1985) developed a hydrologic-economic response model for the Livermore Basin in northern California. The underlying aquifer is a two-layer, unconfined/confined system. They used the response matrix approach coupled with the iterative method to address nonlinear transmissivity in the upper, unconfined layer. Influence coefficients are generated using the transient, quasi-three-dimensional, finite-difference model of Trescott (1976). The iterative approach linearizes the system and iterates a management model containing the linearized system. Others have termed this procedure as cycling. To address stream recharge and well pumping costs approximated by piecewise linear equations, the mixed integer programming was used.
Willis and Yeh (1987) presented a procedure to deal with flow in a small, one-dimensional, unconfined system using a response equation. This nonlinear response equation is a differential equation transformed from the Boussinesq equation (Willis, 1984). The nonlinear response equations are quasi-linearized using the generalized Taylor series. Because of this quasi-linearization, a series of optimizations is needed to achieve a solution of the original unconfined aquifer system.

Elwell and Lall (1988) used the response matrix approach for analyzing groundwater development in the Salt Lake Valley of Utah. They superimposed a two-dimensional finite-difference grid on the area of interest in the unconfined aquifer system. To address the nonlinearity of the unconfined, leaky, or stratified aquifer, the Girinski potential was used instead of head in the management model.

The approach most suitable for a given situation is dependent upon simulation accuracy, flow conditions (steady or unsteady), spatial scale (large-scale or small-scale), and the computational capacity of hardware and software (Gorelick 1983; Peralta et al., 1991b). Peralta et al. (1991b) provided a comparison regarding the required computer memory and the accuracy of the computed results using models designed to develop sustained-yield strategies in a hypothetical confined aquifer (11 x 9 = 99 cells). They concluded that the embedding model requires less computation time and computer memory than the response matrix model if the proportion of
pumping cells and cells requiring head computation or constraints within the optimization is large.

The first objective of this study is to enhance the modelling approach originally presented in USUGWM and to make it completely applicable for fully nonlinear systems and for steady-state condition. The original USUGWM contains both fully and partially linearized models. When the fully linear model is applied to a nonlinear system, heads from the previous cycle are used to compute transmissivity and to select the correct linear segments of equations for evapotranspiration (Et), river-aquifer interflow, and flow reduction. The model is re-optimized until the values of variables do not change with the cycles. In the nonlinear model, the above external flows are represented by their nonlinear formulation, but transmissivity is still treated linearly (Gharbi et al., 1990). When the nonlinear model is applied to an unconfined aquifer, cycling is necessary.

For illustration, now Et, described using piecewise linear equations (segments), is explained below. Et is a known maximum values if the water table elevation in an unconfined aquifer exceeds a certain elevation (proximity to the ground surface). Et is zero if the water table is beneath a certain elevation. Between these two elevations, Et changes linearly from the maximum value to zero. Et is a nonsmooth process because its equation is segmented and not continuously differentiable. To address this problem linearly requires deciding, before optimization, which linear segment of the Et
equation to use.

Because of the pre-selection of the linear segments for nonsmooth external flow functions, the fully linearized model of USUGWM would not necessarily converge to the optimal solution if the initial guess of the solution was far from that optimal solution. To address that problem, a USUGWM user should switch from the fully linearized model to the partially linearized model. In this study, the linearized model is improved so that it will always converge to the same solution regardless of its initial guess.

In addition, a fully nonlinear embedding model, in which transmissivity is represented as a nonlinear function of head, is newly developed. This model directly computes an optimal solution without cycling.

The second objective of this study is to construct a response matrix model so that it has comparable ability to address nonlinear systems as the embedding approaches mentioned above. As described previously, several researchers have applied the response matrix approach to unconfined aquifers. However, none of these models contained external, hydrological flows described by nonsmooth functions such as drain discharge. If the flow equation contains these external flows and they are significant, then superposition cannot be used directly. In this paper, we show how to use linear superposition with cycling to address such nonlinear, nonsmooth flow systems.
The third objective attempts to increase the probability of achieving globally optimal solutions for these nonlinear systems. That involves two issues: (1) It is difficult to prove that the optimal solution to a linear surrogate of a nonlinear problem is also an optimal solution of the original nonlinear problem (Gorelick, 1983; Gharbi and Peralta, 1992). An approach to prove this is to successfully develop the fully nonlinear model and to compare solutions. (2) It is difficult to know whether the solution solved by a nonlinear model is local or global optimal. Here, for a selected system, we demonstrate that three types of embedding models (fully linear, partially linear, and fully nonlinear models) and the response matrix model all achieve the same optimal solution even if the models are run with different initial guesses chosen from a wide range. Empirically, perhaps global optimality is achieved.

The fourth objective is to compare alternative approaches computing sustained-yield pumping strategies for a complex nonlinear aquifer system. Alternatives include three embedding and one response matrix model. These models can replicate all of the steady-state simulation abilities of the USGS modular, three-dimensional, finite-difference, groundwater flow model, MODFLOW, (McDonald and Harbaugh, 1988) while computing optimal groundwater pumping strategies. The embedding models contain finite-difference approximations of a quasi-three-dimensional flow equation as constraints. The response matrix model computes heads using superposition and
influence coefficients, generated by a modified McDonald and Harbaugh (MODFLOW). Also, a predictive technique for deciding which model is most appropriate for a specific situation based on required memory is demonstrated.

To achieve these goals, some definitions are first provided. Then the objective function is presented, followed by a discussion of the four steady-state optimization models being compared. All are tested for a hypothetical three-layer system having unconfined and confined layers, a nonsmooth flow, and six potential pumping cells. Finally memory requirements of each modelling approach are compared.

Iteration and Cycling

The following terms are used in subsequent sections and are defined below:

**Iteration**

An iteration refers to the processing of solvers, such as the LP and DNLP solvers in the MINOS optimization software and the SIP (Strong Implicit Package) solver in MODFLOW. Many iterations might be required to find a solution.

**Cycling**

Cycling is a recursive process of solving an optimization problem over and over. Between cycles, changes are made in assumed parameter values on utilized equations. For example, first, nonlinear formulas are linearized. Then the model containing the linearized formulas is optimized using initial guesses of variables. For the
second cycle, parameters are recomputed, and the optimization model is rerun. The process of using the optimal solution from the previous run to initialize parameter values for the next optimization is repeated until the computed optimal variable values do not change with the cycles. Here, nonlinear terms include transmissivity in an unconfined aquifer and use external flows described by nonsmooth functions. For all presented models, except for the fully nonlinear embedding model, multiple cycles are usually required to achieve the true optimal solution when the models are applied to flow systems including a unconfined aquifer and/or nonsmooth functions.

Models Using Embedding Approach

In this section, three alternatives are presented. Alternatives E1 and E2 are prepared using the USU groundwater management model (USUGWM) initially developed for the Salt Lake Valley (Gharbi et al., 1990) but modified with the added ability to address flowing (artesian) wells (Takahashi and Peralta, 1991). Alternative E1 is fully linear. Alternative E2 is nonlinear for nonsmooth external flows but linear for transmissivity. Alternative E3 is a newly demonstrated fully nonlinear model which requires neither linearization nor the cycling procedure. All these models are written in General
Algebraic Modeling System, GAMS (Brooke et al., 1988). Optimizations are performed using MINOS (Murtagh and Saunders, 1987).

**Model Formulation**

**Objective Function**

The objective function of each model is to maximize total steady groundwater extraction.

$$\text{maximize } z = \sum_{o=1}^{N} g_{p_o}$$

where

- $g_{p_o}$ groundwater pumping in cell $o$ located in layer 1, row $i$, and column $j$, $(L^3/T)$;
- $N$ total number of cells with potential pumping wells.

In the model, discharge, i.e. groundwater pumping, is a positive value, and recharge is a negative value.

**Constraints Describing the Physical Flow System**

The steady-state, finite-difference form of the quasi-three-dimensional groundwater flow equation (McDonald and Harbaugh, 1988) is used as constraints (one for each cell and layer).

$$CR_{i,j+1/2}(H_{i,j+1} - H_{i,j}) + CR_{i,j-1/2}(H_{i,j+1} - H_{i,j}) +$$
$$+ CC_{i+1/2,j}(H_{i+1,j} - H_{i,j}) + CC_{i-1/2,j}(H_{i-1,j} - H_{i,j}) +$$
$$+ CV_{i+1/2,j}(H_{i+1,j} - H_{i,j}) + CV_{i-1/2,j}(H_{i-1,j} - H_{i,j})$$

$$= \sum_{n=1}^{N} q_{i,j,n}$$

(2)
where

\[
\begin{align*}
CR_{l,i,j+1/2} &= 2dx_j (T_{l,i,j}^{i-1} / (T_{l,i,j}^{i} T_{l,i,j+1}^{i+1})) \tag{3a} \\
CC_{l,i+1/2,j} &= 2dy_i (T_{l,i,j}^{i-1} / (T_{l,i,j}^{i} T_{l,i+1,j}^{i+1})) \tag{3b} \\
CV_{l+1/2,j} &= dx_j dy_i / \{ (dz_1 / 2K_{l,i,j}) + (dz_{l+1} / 2K_{l+1,i,j}) \} \tag{3c}
\end{align*}
\]

\(H_{l,i,j}\) potentiometric head, \((L)\);

\(T_{l,i,j}\) transmissivity, \((L^2/T)\);

\(l,i,j\) layer, row, column indices of a finite-difference cell;

\(CR, CC\) hydraulic conductances (harmonic averages of transmissivities) along \(x, y\) axes between the nodes, \((L^2/T)\);

\(CV\) vertical conductance between the nodes, \((L^2/T)\);

\(dx, dy, dz\) cell sizes in layer \(l\), row \(i\), and column \(j\), \((L)\);

\(K_{l,i,j}\) vertical hydraulic conductivity, \((L^2/T)\);

\(q_{l,i,j,n}^*\) \((n\text{th})\) external flow term in a cell, \((L^3/T)\).

**Alternatives E1 and E2.** For a confined layer, transmissivity is constant. Thus, hydraulic conductances \(CR, CC,\) and \(CV\) are constant, and the left-hand side (LHS) of Equation 2 is always linear. For an unconfined layer, transmissivity should most properly be a function of an unknown head and hydraulic conductivity \((T = kh)\). In Alternatives E1 and E2, transmissivity \((T_{l,i,j} = k_{l,i,j} HFC_{l,i,j}^{n-1})\) is constant in a cycle by substituting a head \(HFC_{l,i,j}^{n-1}\) known from the former \((n-1)\) cycle for an unknown head \(H\) in the present cycle. Thus, hydraulic conductances \(CR, CC,\) and \(CV\) are constant, and the LHS of Equation 2 becomes linear in each cycle. Cycling
is continued until heads do not change with the cycles. Alternative E1 requires cycling to treat the nonsmooth flows and transmissivity of an unconfined aquifer. E2 uses cycling only to address transmissivity.

Alternative E3. For a confined aquifer, transmissivity is constant as in Alternatives E1 and E2. For an unconfined aquifer, $T_{ij} = K_{ij} H_{ij}$ and one uses an unknown head $H$. As a result, hydraulic conductances $CR$ and $CC$ are nonlinear while $CV$ is always linear. The LHS of Equation 2 is nonlinear.

The models also compute various external flow terms: (1) flow at sources or sinks such as pumping/recharge wells ($qp$), drains ($q^d$), or flowing wells ($q^f$), (2) other processes such as stream-aquifer interflow ($q'$), flow across a general head boundary ($q^g$), evapotranspiration ($q^e$), flow reduction due to partial desaturation ($q^ro$), areal constant recharge ($q^r$), and flux across constant head boundary ($q^c$).

All external flows except for $q'$ are treated as variables. External flows dependent on head in the subject cell are formulated separately from the flow equation (Equation 2) as independent constraints. Based on their formula (linear or nonsmooth and dependent or independent of head), those external flow terms are classified into three types. This is important for subsequent explanations because the model development and solving procedure differ with each type.

Type 1. These external flows are assumed to be independent of groundwater head in the subject cell or to be dependent on a constant head.
gp_{i,j} \quad \text{pumping rate in a cell, } (L^3/T);

q'_{i,j} \quad \text{saturated flow across a constant head boundary cell, } (L^3/T);

q''_{i,j} \quad \text{known constant recharge in a cell, which includes bedrock recharge, unsaturated canal seepage, irrigation seepage, precipitation in the recharge area, } (L^3/T).

\text{Type 2. This external flow is represented by a linear function of head in the subject cell.}

- \text{Recharge/discharge through general head boundary for all alternatives:}

\begin{align*}
q''_{i,j} &= \text{saturated flow between the aquifer and a general head boundary in the cell, } (L^3/T); \\
&= \Gamma'^{s}_{i,j} (H_{i,j} - h^k_{i,j}) \quad (4)
\end{align*}

where

- \Gamma'^{s} \quad \text{hydraulic conductance between the aquifer and general head boundary cell, } (L^2/T);

- h^k \quad \text{fixed water level such as that of the sea, } (L).

\text{Type 3. These external flows are assumed to be represented by a nonsmooth function of head in the subject cell. The function consists of two or three linear segments. For Alternative E1, the segment to be used is based on head from the previous cycle. In Alternatives E2 and E3, these flows are solved using } (\max \text{ or } \min (\text{argument 1, argument 2}))\text{, a DNLP (nonlinear programming with discontinuous derivatives) option of MINOS.}
Discharge from drains

for Alternative E1:

\[ q^d_{i,j} = \text{saturated flow leaving the aquifer in a cell with drains, } (L^3/T); \]

\[ = R^d_{i,j}(H_{i,j} - B^d_{i,j}) \quad \text{for } HFC^d_{i,j} > B^d_{i,j} \]

\[ = 0 \quad \text{for } HFC^d_{i,j} < B^d_{i,j} \quad (5a) \]

for Alternatives E2 and E3:

\[ q^d_{i,j} = R^d_{i,j} \max(H_{i,j} - d_{i,j}, 0) \quad (5b) \]

where

- \( R^d \) hydraulic conductance between the aquifer and drains, \((L^2/T)\);
- \( B^d \) Bottom elevation of the drains, \((L)\).

In 5(a), if a head \( HFC \) known from the former cycle is above the drain bottom \((HFC > d)\), then \( q^d = R^d(H-d) \), otherwise \((HFC \leq 0)\), \( q^d = 0 \). Since the linear segment is not selected using an unknown head \( H \) in the current cycle, this linear formula needs cycling to solve drain discharge.

In 5(b), the \( \max(H_{i,j} - d_{i,j}, 0) \) selects the bigger of \((H_{i,j} - d_{i,j})\) and 0 while simultaneously performing the optimization. If an unknown head \((H)\) in the current cycle is above the drain bottom \((H \geq d)\), then \( q^d = R^d(H-d) \), otherwise \((H < d)\), \( q^d = 0 \). Thus, cycling is not necessary to solve this formula (Gharbi et al. 1990). Other Type 3 external flows are also solved in the same manner as this.
- **Evapotranspiration**

for Alternative E1 (Linear formula):

\[ q_{l,ij} = \text{distributed discharge from evapotranspiration in a cell, (L}^3/\text{T);} \]

\[ = E_0 \, dx_i dy_i \quad \text{for } \text{HFC}_{l,ij} > h'_{l,ij} \]

\[ = E_0 \, dx_i dy_i \left\{ H_{l,ij} - (h'_{l,ij} - d_{l,ij}) \right\}/d_{l,ij} \]

\[ \quad \text{for } h'_{l,ij} - d_{l,ij} < \text{HFC}_{l,ij} < h'_{l,ij} \]

\[ = 0 \quad \text{for } \text{HFC}_{l,ij} < h_{s,ij} - d_{l,ij} \quad (6a) \]

for Alternatives E2 and E3 (DNLP formula):

\[ q_{l,ij} = E_0 \, dx_i dy_i/d \]

\[ \{ \min(h'_{l,ij}, H_{l,ij}) - \min(h_{l,ij} - d_{l,ij}, H_{l,ij}) \} \quad (6b) \]

where

- \( E_0 \) potential evapotranspiration, (L/T);
- \( h' \) potentiometric surface elevation below which evapotranspiration decreases, (L);
- \( d \) extinction depth, (L);

- **Discharge from flowing wells**

for Alternative E1:

\[ q_{l,ij} = \text{discharge from flowing wells or springs in a cell, (L}^3/\text{T);} \]

\[ = \Gamma_{l,ij} \, (H_{l,ij} - h'_{l,ij}) \quad \text{for } \text{HFC}_{l,ij} > h_{s,ij} \]

\[ = 0 \quad \text{for } \text{HFC}_{l,ij} < h_{s,ij} \quad (7a) \]

for Alternatives E2 and E3:

\[ q_{l,ij} = \Gamma_{l,ij} \cdot \max(H_{l,ij} - h'_{l,ij}, 0) \quad (7b) \]

where

- \( \Gamma \) coefficient describing reduction in discharge rate
of the flowing wells per 1 foot head decline, 
\( (L^2/T) \);

\( \text{h}_g \) ground surface, \( (L) \).

- **Stream-aquifer interflow**

  for Alternative E1:

\[ q'_{i,j} = \text{interflow between the aquifer and stream in a} \]
\[ \text{selected river cell, } (L^2/T); \]

  for saturated flow

\[ = \Gamma_{i,j}^s (H_{i,j}-\sigma_{i,j}) \]
\[ \text{for } HFC_{i,j}^a > B_{i,j}^b \]

  for unsaturated flow

\[ = \Gamma_{i,j}^u (B_{i,j}-\sigma_{i,j}) \]
\[ \text{for } HFC_{i,j}^a < B_{i,j}^b \]  \( \text{(8a)} \)

for Alternatives E2 and E3:

\[ q''_{i,j} = \Gamma_{i,j}^a \max(H_{i,j}-\sigma_{i,j},B_{i,j}-\sigma_{i,j}) \]  \( \text{(8b)} \)

where

\( \Gamma^d \) hydraulic conductance between the aquifer and river, 
\( (L^2/T) \);

\( \sigma \) elevation of the free water surface in the river, 
\( (L) \);

\( B^b \) bottom elevation of the river, \( (L) \).

If an elevation of the free water surface in the river can be assumed to be constant, then \( q' \) is constant for unsaturated flow.

- **Vertical flow reduction**

  for Alternative E1:

\[ q'_{i,j}^d = \text{vertical flow reduction to correct overestimation} \]
\[ \text{in Equation 2 when the lower confined aquifer is} \]
\[ \text{desaturated } (L^3/T); \]
for Alternatives E2 and E3:

\[ q_{d,ij} = - CV_{i,j} \max (H_{i,j} - E_{top}^{i+1,j}, 0) \]  

(9b)

where

\[ E_{top}^{i+1} \] elevation of the top of layer \( l+1 \), (L);

Bounds on Variables

For all three alternatives, bounds on pumping rate and head are described as:

\[ h_{L,ij} \leq h_{i,j} \leq h_{U,ij} \]  

(10)

\[ gp_{L,ij} \leq gp_{i,j} \leq gp_{U,ij} \]  

(11)

where

\[ L, U \] denote lower and upper bounds, respectively.

Usually, bounds on head are used to avoid or minimize problems caused by unacceptable drawdowns, while bounds on pumping are set based on a well capacity and/or water demand. Other bounds can be added depending on the problem. For example, if flux across the constant head boundary must be restrained, the bounds are described as:

\[ q_{L,ij}^{e} \leq q_{i,j}^{e} \leq q_{U,ij}^{e} \]  

(12)

Solution Procedures

The steady-state finite-difference form of the quasi-three-dimensional groundwater flow equation (McDonald and Harbaugh, 1988) contains the following: (1) nonlinearity in an unconfined aquifer, where transmissivity is not constant but
is a function of head, and (2) Type 3 external flows. These terms cannot be solved with the LP technique directly or without additional action. In Alternatives E1 and E2, the fully and partially linearized models, respectively, are formulated first. To achieve an optimal solution to a linear surrogate of a nonlinear problem, the models are solved repeatedly until variable values do not change with the cycles (Gharbi et al., 1990). In Alternative E3, the above terms are formulated in a nonlinear manner and are solved using the MINOS DNLP solver without the cycling procedure. Flow charts of solution procedures for the models are shown in Figure 1 and are described below.

**Alternative E1**

1. Read and prepare: read data files and set heads in the first cycle \((HFC^0)\) equal to starting heads \((STRT)\) which are initially guessed or given.

2. Formulate (start of cycle): using heads in the former \((n-1\text{th})\) cycle \((HFC^{n-1})\), estimate the transmissivity \((T)\) and conductances \((CR, CC, \text{ and } CV)\) and determine the linear segment of each Type 3 external flow. As a result, the transmissivity and conductances become constant. Additionally, the external flow is described as either \((aH-b)\) or \(b\) \((a \text{ and } b \text{ are constant and } H \text{ is variable})\). For example, drain discharge \(q^d\) is either (conductance \((\Gamma^d)\) x unknown head \((H)\) - \(\Gamma^d \times B^d\) (drain bottom) or 0. Thus, the flow equation (Equation 2) and
external flows become linear.

3. Solve: using the MINOS LP solver, solve the linear model, which includes the flow equation (Equation 2) and external flow linearized in step 2 as constraints. The LP solver uses an advanced simplex method. To commence, set initial values of head (H) equal to $H_{FC}^{-1}$.

4. Compare and converge (end of cycle): compare optimal solutions of variables such as head and pumping rate in the current (n th) cycle and those in the former (n-1 th) cycle. If the difference between the optimal solutions of two consecutive cycles satisfies criteria which indicate convergence of the variables, then go to step 6; otherwise, go to step 5.

5. Replace: the optimal solutions in the former (n-1 th) cycle are replaced with those in the current (n th) cycle. Go back to step 2 and continue through step 4.

6. Optimal solution: stop the cycle, and the true optimal solutions are found.

**Alternative E2**

The solving procedure of Alternative E2 is the same as Alternative E1 except for steps 2 and 3 which are described below.

2. Formulate (start of cycle): using heads in the former (n-1 th) cycle ($H_{FC}^{-1}$), estimate transmissivities ($T$) and conductances ($CR$, $CC$, and $CV$).

3. Solve: using the MINOS DNLP solver, solve the model,
which includes the flow equation (Equation 2) linearized only with respect to transmissivities in step 2 and DNLP formulas of Type 3 external flows as constraints. The DNLP solver uses a reduced gradient method.

**Alternative E3**

1. Read and prepare: read data files including starting heads (STRT).

2. Formulate: using starting heads, estimate the transmissivity and hydraulic conductances (CRstrt and CCstrt).

3. Solve: using the MINOS DNLP solver, solve the nonlinear model, which includes the nonlinear formula of the flow equation (Equation 2) and DNLP formulas of Type 3 external flow terms as constraints. In the system, initial values of H and the conductances (CR.L and CC.L) are set equal to STRT, CRstrt, and CCstrt, respectively.

4. Optimal solution: the true optimal solutions are found.

In Alternative E3, the nonlinearities are formulated more ideally than in Alternatives E1 and E2. However, because of its nonlinearity, more memory and more strict programming requirements are necessary. These include better conception of an initial guess and bounds.

If Alternatives E1 and E2 are applied to a completely linear flow system, which includes neither an unconfined aquifer nor type 3 external flows, then the cycling procedure is skipped.
Global Optimality

The optimal solution of the fully linear model (E1 and a response matrix model) is globally optimal. However, it uses cycling, and the global optimality is guaranteed only in each cycle. On the other hand, the fully nonlinear model (E3) does not use cycling, but the DNLP solver looks for the local optimal solution. There are two problems concerning the optimality. First, it is difficult to know if the optimal solution to a linear surrogate of a nonlinear problem via cycling (in E1 or E2) is the solution of the original nonlinear problem (E3). Second, it is uncertain that the solution of nonlinear models (E2 or E3) is unique (globally optimal), meaning that a better solution exists. If the presented nonlinear problem is convex, it has only one optimal solution, the global optimum. In that case, all these models should achieve the same optimal solution.

Model Using Response Matrix Approach: Alternative RM

A response matrix model which can simulate groundwater flow in a complex nonlinear aquifer system using the principle of superposition is presented here. This alternative uses influence coefficients generated by a modified version of the MODFLOW model written by McDonald and Harbaugh (1988). The management models are written in GAMS and are solved with the MINOS LP solver.

The basic idea in solving the nonlinear flow system is the same as Alternative E1 except that superposition rather
than embedding is used to compute heads. In this case, the flow equation (Equation 2) and constraints describing Type 3 external flows are treated linearly in each cycle and superposition is used. The cycling procedure is still used to ensure that final optimal equation segments and transmissivities are the same as those assumed commencing the cycle.

The size of the management model can be reduced drastically in some cases by using the response matrix approach instead of the embedding approach. To facilitate the use of the response matrix approach for nonlinear flow systems, MODFLOW is converted and modified into two independent external simulation models termed the Pre-Influence Coefficient Generator (Pre-ICG) and the Influence Coefficient Generator (ICG). The ICG is used to generate influence coefficients. The Pre-ICG computes heads for the ICG in the next (n+1) cycle.

**Modified McDonald and Harbaugh (MODFLOW) Models**

The objective is to gain the ability to use linear influence coefficients, superposition, and cycling to accurately represent head response to stimulus in a nonlinear system (unconfined aquifer and Type 3 external flow equations). The approach is presented after reviewing how the original MODFLOW works.

MODFLOW uses only linear equations. It selects which Type 3 equation segment (and transmissivity) to use based on
values at the beginning of an iteration. Then it solves for those external fluxes based on their segments. Next, MODFLOW solves the entire flow equation with those external fluxes as knowns. There are many iterations and segment selections before convergence to a solution.

Since we are using MODFLOW to generate influence coefficients, we must achieve compatibility between the management model and MODFLOW. To do this, assumptions used within a cycle of optimization modelling must be the same as those used in a single iteration in MODFLOW. Otherwise, convergence of solution would not always occur.

After using the same assumptions in developing influence coefficients and in subsequently computing the optimal strategy, some of the assumed equation segments of Type 3 external flows will be wrong (for the optimal pumping rates, although they are correct for the utilized unit pumping rates). However, segment assumptions will be corrected through cycling just as MODFLOW corrects these equations through iteration.

**Pre-Influence Coefficient Generator (Pre-ICG)**

The purpose of the Pre-ICG is to compute the heads needed by the ICG to calculate transmissivities and influence coefficients for the next cycle. Before describing how the Pre-ICG works, we present the common techniques used in normal simulation modelling.

**Type A:** Transmissivity is assumed constant through all
time steps if the drawdown in an unconfined layer is relatively small compared with the saturated thickness. Less than 10% change in saturated thickness is usually acceptable for assuming system linearity (Reilly et al., 1987).

Type B: Transmissivity is assumed constant for each time step but is recomputed at the end of each time step. If this technique is applied to the steady-state, it is similar to Type A because a steady-state simulation uses either no time step (Storage coefficient = 0) or only one very long time step.

Type C: Most groundwater flow simulation models, including MODFLOW, rely on iterative methods to solve the flow equation. These address the nonlinearity of an unconfined aquifer more realistically than the above techniques because transmissivity is assumed constant only in each iteration rather than in each time step. (There are many iterations within a time step).

MODFLOW's steady-state solution procedure for nonlinear aquifer systems is discussed and shown in Figure 2(a). The steps are:

1. Read and prepare: read data files and set heads (HOLD) in the first time step (there is only one pseudo-time step for steady-state) equal to starting heads (STRT).
2. Prepare for iteration: set heads in the first iteration (HNEW0) equal to HOLD.
3. Formulate (start of iteration): determine transmissivity (T), conductances (CR, CC, and CV), and external flow
terms using heads in the former \((m-1)\) iteration \(H_{\text{NEW}^{m-1}}\) for each node. As a result, the transmissivity and conductances are constant within an iteration. Additionally, the external flow term is described as either \((a \times H_{\text{NEW}^m} - b)\) or \(b\) \((a\) and \(b\) are constant and \(H_{\text{NEW}}\) is variable). Equation 2 is linear here.

4. Solve: compute a solution to the flow equation linearized in step 3 with one of the alternative solvers such as Strong Implicit Procedure (SIP), a method for solving a large system of simultaneous linear equations by iteration.

5. Close (end of iteration): iteration proceeds until closure achieves \((\text{maximum } (H_{\text{NEW}^m} - H_{\text{NEW}^{m-1}}) \leq \text{specified convergence criteria})\).

6. Final solution.

Type D: Another simulation procedure, which combines Type B and MODFLOW's simulation procedure to involve the LP technique in the management model, was used in USUGWM (Gharbi et al. 1990). In using USUGWM for transient optimization, transmissivity is estimated using hydraulic conductivity and optimal time varying head from the former cycle. As in Type B, transmissivity is assumed constant within a time step. However, transmissivity is recomputed for all time steps at the end of each cycle. This procedure is continued until transient heads do not change with the cycles. The simulation results of the USUGWM have been virtually identical to those of the MODFLOW.
In this study, MODFLOW is modified to be compatible with a Type D approach for steady-state. The solution procedure is presented in Figure 2(b) and is described as follows:

1. Read and prepare for time step: read data files and set heads (HOLD) in the first time step (but only one pseudo-time step for steady-state) to starting heads (STRT).
2. Prepare for cycle: set heads in the first cycling loop (HFC⁰) to HOLD.
3. Formulate (start of cycle): determine transmissivity (T), conductances (CR, CC, and CV) and external flow terms using heads in the former (n-1 th) cycle HFCⁿ⁻¹. As a result, transmissivity and conductances become constant. Additionally, the external flow term is either (a x HNEWⁿ - b) or b. Equation 2 is linear here.
4. Prepare for iteration (start of iteration): set heads in the first iteration (HNEW⁰) equal to HFC⁰⁻¹.
5. Solve: compute a solution to the linear equation in step 3 using a solver such as SIP.
6. Close (end of iteration): iteration proceeds until closure achieves (maximum (HNEWⁿ-HNEWⁿ⁻¹)) ≤ specified convergence criteria.
7. Set heads in the current cycle (HFCⁿ) equal to heads solved through the iteration (HNEWⁿ).
8. Converge (end of cycle): cycling procedure proceeds until closure achieves (maximum (HFCⁿ-HFCⁿ⁻¹)) ≤ specified convergence criteria.
Influence Coefficient Generator (ICG)

MODFLOW, in which the flow equation is linear at the beginning of each iteration, cannot be used directly as the Influence Coefficient Generator (ICG) for nonlinear flow systems. The ICG generates influence coefficients at the beginning of each cycle and is designed to perform as described below:

a. Read data files using mostly MODFLOW format. Added is a file identifying those cells for which head has to be computed within the optimization model.

b. Using SIP to generate influence coefficients for the entire system, solve the flow equation linearized at the beginning of each cycle.

c. Make a response matrix table containing influence coefficients.

The ICG calculates:

$h_{um}$ Unmanaged head describing average head response over a cell $o$ to known steady stresses (bed rock recharge, precipitation, etc.), ($T/L^2$);

$\delta_{o,m}$ Influence coefficient describing the average head response at cell $o$ to a unit pumping in cell $m$, ($T/L^2$).

Computation of Head Using Influence Coefficients

The summation of influence coefficients times pumping is contained in the management model as a constraint to compute heads in specific cells.
\[ h_o = h_{um}^o + \sum_{m=1}^{N} \delta_{o,m} q_m \]  \hspace{1cm} (13)

where

- \( h_o \) average potentiometric head in cell \( o \), (L);
- \( q_m \) unit pumping in cell \( m \), (L³/T).

**Model Formulation**

The objective function and bounds on variables of the response matrix approach are the same as in the embedding models. Their different forms are its constraints describing head. These are used only for specific cells, as opposed to being used for all cells as in the embedding approach.

**Constraints Describing the Physical Flow System**

To apply superposition and cycling to the nonlinear system and to calculate external flows, the following cell types are defined:

- **VHCf** variable head cell containing external flows which are functions of head.
- **VHCb** variable head cell in which head must be bounded to prevent unacceptable drawdown, salt-water intrusion, or other problems.

Equation 13 is used to compute head only for VHCb. External flows are computed externally by running the Pre-ICG with optimal pumping. However, if some external flows are bounded, Equation 13 is used for VHCf. Types 2 and 3 external flows are dependent on head in the subject cell. Those flows
are used and independently formulated only if they require constraint.

Solution Procedures

A solution procedure of Alternative RM is shown in Figure 3.

Alternative RM

In the management model:

1. Read and prepare: read data files and set heads (HFC\(^0\)) in the first cycle loop equal to starting heads (STRT) which are initially guessed or given.

In the ICG:

2. Run external ICG: run an external Influence Coefficient Generator (ICG) using heads of the unconfined aquifer in the former (n-1 th) cycle (HFC\(^{n-1}\)).

In the management model:


4. Formulate (start of cycling loop): using heads (HFC\(^{n-1}\)) in the former (n-1 th) cycle, estimate transmissivities and hydraulic conductances and determine which linear segment of Type 3 external flow is applied.

5. Solve: using the MINOS LP solver, solve the linear model which includes superposition (Equation 13), Type 2 external flow, and LP formulas of Type 3 external flows which are linearized in the former steps. In the model, an initial value of H is set equal to HFC\(^{n-1}\).
6. Compare and converge (end of cycle): compare optimal values of variables such as head and pumping rate in the current (n th) cycle and those in the former (n-1 th) cycle. If the difference between the optimal solutions of two consecutive cycles satisfies certain criteria which indicates the convergence of variables, then go to step 8; otherwise, go to step 7.

7. Run external Pre-ICG: using optimal pumping rate in the current (n th) cycle and heads in the former (n-1 th) cycle HFc•-1, run Pre-ICG to re-estimate heads needed to recompute the transmissivities (T) and conductances (CR and CC) of the unconfined aquifer for the next (n+1 th) cycle optimization.

8. Replace: optimal solutions of heads and variables of the former cycle are replaced with heads resulting from Pre-ICG and optimal solutions of the current (n th) cycle.

9. Optimal solution: stop the cycle, and the true optimal solutions are found.

In summary, solution procedures and formulas in all the management models are shown in Table 1. The embedding models do not use external programs such as the ICG. On the other hand, the response matrix model uses both the ICG and the Pre-ICG.

Model Application

The sample problem is addressed for a hypothetical three-layer aquifer system using all four alternatives. The aquifer
system has the following complicating characteristics: (1) multilayer, (2) unconfined and confined aquifers, and (3) Type 3 external flow.

**Hypothetical, Three-Layer Aquifer System**

Consider the hypothetical three-layer aquifer system of Figure 4 (McDonald and Harbaugh, 1988). The upper layer is unconfined, the middle and lower layers are confined, separated from each other by aquitards. The aquifer is square measuring 75,000 ft on a side, and is discretized into 625 cells (3 layers x 15 rows x 15 columns). Flow within the aquitards is not simulated, but vertical flow between the layers is computed using vertical conductances. Flow into the system is through infiltration from precipitation. Flow leaves the system via six pumping wells, drains, and the sea, represented by a constant head boundary. Initial heads in Layer 1 range from zero at a constant boundary to 178.90 ft at both corners furthest from the sea.

**Description of Scenario**

The problem objective is to maximize total sustainable (steady-state) groundwater pumping subject to hydraulic constraints. Six pumping cells are located in the lowest layer. Upper and lower bounds on pumping rates are 16 cfs and 4 cfs, respectively. The lower bound on head at the pumping cells is 30 ft above sea level.
Model Formulation

The embedding models are formulated as shown in Table 2. In Alternative RM, heads of the unconfined aquifer, needed to estimate transmissivity in the next cycle, are estimated using the Pre-ICG. Only heads in six pumping cells are estimated with Equation 13. Flow across constant head boundary \((q^c)\) and drain discharge \((q^d)\) are estimated using the Pre-ICG.

Results

Initially assumed heads are 0.0 ft in all cells. This initial guess is intentionally chosen to be far from the optimal head to rigorously test the models' ability to always reach the same optimal solution. For E1 and E2, the optimization continues cyclically until the largest absolute difference between heads for two consecutive cycles is less than 0.001 ft. This requires six cycles. Response matrix model RM is also cycled six times. The resulting optimal aquifer water budgets for all embedding models include 157.500 cfs precipitation, 69.030 cfs pumping, 36.745 cfs flow from drains, and 51.725 cfs flow to the sea. There was no error in the volume balance for all the models. Fluxes for the response matrix model was within 0.002 cfs of the above rates. The optimal potentiometric head in Layer 3 is shown in Figure 5.

The fully nonlinear model (E3) calculates the same solution as the other models, even when radically different initial guesses are chosen. Global optimality seems to be
obtained.

Computational Accuracy

Because E3 does not use any linearization before beginning the solution, it solves the nonlinear flow system most accurately of all the models. E1 and E2 achieve the same optimal results as E3 by cycling. The final optimal solutions in the response matrix model also are virtually identical to those of E3. However, the computational accuracy of a response matrix model depends on how appropriately influence coefficients are generated with external simulation models. In the sample problem, 1 cfs is used as a unit pumping and the following SIP parameters are specified: (a) the error criteria: 0.0001 ft, (b) the acceleration parameter: 1.0, (c) the maximum number of iterations: 200, (d) the seed: 0.001, (e) the number of iteration parameters 100, and (f) the head change criteria: 1.0. The ICG needs about 30 iterations to generate a set of influence coefficients for one unit pumping. The number of significant figures also affects the accuracy. To obtain optimal values acceptably close to those of E3, the influence coefficients have four digits after the decimal point (i.e., 2.2345 (ft s/ft³)).

Other combinations of SIP parameters and unit pumping or use of other solvers may converge more quickly and yield more accurate results than those obtained here. However, searching for the best combination of SIP parameters and unit pumping involves trial and error. Since RM uses two external
simulation models, its errors in computing heads might be greater unless its unit pumping and SIP parameters were well chosen.

**Computational Efficiency**

Because MINOS itself has no fixed limit on the size of a problem, a limiting factor is the amount of main storage available on a particular machine and CPU time which is shared for a decision-maker (Brooke et al, 1988). Therefore, it is important to know a priori the size of an optimization scheme required to implement a particular modelling approach for a specific aquifer problem.

The number of equations, variables, and nonzero elements indicates the size of the optimization model. A coefficient related to a linear term is a linear nonzero element (otherwise, a nonlinear, nonzero element). The number of equations and variables equals the number of rows and columns in the solved matrix, respectively. However, unless most cells are pumping cells and locations of head constraint, most of the matrices are sparse. In fact, most elements in the matrices are zero. To avoid occupying main storage with such a large number of zeros, MINOS uses one large array to store only nonzero elements in main storage (Brooke et al., 1988). If a nonlinear formula is involved, additional memory is required. The number of nonlinear elements shows the degree of nonlinearity.
The number of equations, variables, and nonzero elements can be predicted by counting the number of constraints and the number of variables and coefficients in those constraints. For example, in Alternative E2, using the embedding method, out of 685 equations, there are 675 flow equations (Equation 2), because each cell contains its own flow equation. The remaining 10 equations include 9 drain discharge equations (Equation 7a), and 1 objective function (Equation 1). Of 721 variables, there are 675 heads (H), 9 drain discharge (qd), 30 fluxes (q^f) at constant head cells, 6 pumping (gp), and 1 objective value (obj). The total number of nonzero elements equals 4,165, including 4,095 hydraulic conductances (CR, CC, and CV), 30 coefficients for q^f's, 9 for q^d's, 6 for gp's in the flow equation (Equation 2), 9 linear and 9 nonlinear nonzero elements in the drain discharge equation (Equation 7b: DNLP formula) and 7 in the objective function (Equation 1).

In Alternative RM, a specific cell contains the superposition (Equation 13). Of the 7 equations, 6 are Equation 13, and 1 is a objective function. Of the 13 variables, there are 6 heads (H), 6 pumping (gp), and 1 objective value (obj). Out of 49 nonzero elements, there are 7 (1+Ngp, Ngp: a number of pumping wells) in the objective function, and (1+Ngp) x (a number of cells with Equation 13: 6) = 42 in the superposition (Equation 13).

Table 4 compares alternative models with respect to computational resource requirement. Included are the number of equations, variables, and nonzero elements, required
memory, consumed CPU time, and cycles to convergence. Some numbers will not change even if the model is run on different machines. On the other hand, required memory and CPU time will vary depending on the machine. We used a VAX 5420. The required CPU time is the total CPU time for six cycles including the time for generating influence coefficients.

In overview, Alternative E3 needs the most memory because of its nonlinearity. Alternative RM needs the least memory because it uses superposition and does not compute heads not needing constraint. On the other hand, Alternative E3 needs the least total CPU time because it avoids cycles. Alternative RM needs the most CPU time because it cycles and uses two external FORTRAN programs.

Prediction of Model Size

In the sample problem having six pumping cells, the response matrix model needs less memory than the embedding models. However, this is not always the result. Memory requirements are situation dependent and can be predicted based on the number of nonzero elements required for the models (Peralta et al., 1991b). The number of nonzero elements is very dependent upon the number of pumping cells and cells requiring head constraint.

In this case, different situations are considered by increasing the number of pumping cells. In comparison, equations for estimating nonzero elements by increasing the number of pumping cells for the hypothetical area system are
shown in Table 5.

In the embedding models, every cell contains the flow equation. Adding a pumping variable to an existing cell adds two linear nonzero elements, one in the flow equation and one in the objective function.

In the response matrix model, required heads are calculated by summation using influence coefficients (Equation 13). In general, nonzero elements are added according to an arithmetic series:

\[ INC_{nz} = \frac{1}{2} NP_t \left( N_h + (NP_t - 1) d \right) \]  

(14)

where

- \( INC_{nz} \) increase in number of nonzero elements.
- \( NP_t \) total number of pumping cells.
- \( d = 2 \)
- \( N_h \) number of cells which are VHCf and VHCB.

This increment can be reduced somewhat if a pumping cell is also a VHCf cell. If pumping cells are installed in the confined aquifer of this hypothetical area, Alternative RM needs the least memory if the problem has 1 to 64 pumping cells. However, in the later case, the ICG must be rerun 64 times. On the other hand, E1 needs the least memory if there are more than 65 pumping cells.

**Summary and Conclusions**

Alternative steady-state groundwater simulation/optimization models for a multilayer, nonlinear, aquifer
system are presented. The models are demonstrated for a rectangular, hypothetical, unconfined/confined aquifer system. The models' objective is to maximize sustained-yield pumping. Constraints include a steady-state, quasi-three-dimensional flow equation and a drain discharge equation. Variables are heads, pumping rate, flux across constant head boundary, and drain discharge. The models are compared with regard to computational accuracy and efficiency. Conclusions are:

1. The E3 fully nonlinear embedding model can compute a correct optimal pumping strategy for an unconfined aquifer without recomputing transmissivities. All other embedding and response matrix models require cycling to recompute transmissivity. The model describes the nonlinear flow system by expressing transmissivities of the unconfined aquifer as a function of heads.

2. The E1 (fully linear) and E2 (nonlinear except for transmissivity) embedding models use cycling to achieve the same solution as the E3 model. These require more solution time but less computer memory.

3. The R3 model uses the principle of superposition instead of the embedding approach. These models can handle external flows via nonsmooth functions as well as transmissivity in an unconfined aquifer. Normal response matrix models cannot solve such nonlinear flow systems because the above terms are not represented by linear equations. This difficulty is overcome by using cycling and linear influence coefficients generated by a modified
McDonald and Harbaugh model (MODFLOW). The accuracy of the optimal solutions depends on how accurately influence coefficients can be computed using the external simulation model.

4. For the tested scenario, the fully nonlinear model (E3) computes the same optimal solution as the other models. It suggested that global optimality is obtained. The tested aquifer system is complex and nonlinear. System components include (1) an unconfined layer where transmissivity is a function of head, (2) drain discharge described by a nonsmooth function, and (3) a three-layer system (675 cells).

5. In the sample problem containing only six pumping cells, the response matrix model (RM) requires less memory than the embedding models. However, if many heads and external flows must be constrained and many potential pumping cells exist, the embedding models are preferred to the response matrix model because of computational efficiency and the ease of obtaining an accurate solution. For the tested system, if more than 65 cells (about 10% of all cells) have pumping potential decision variables, the E1 fully nonlinear embedding model needs the least computer memory. Otherwise, the response matrix model (RM) requires the least memory.

6. In overview, if there is enough available computer memory, the E3 fully nonlinear model is preferred to other models because it can directly achieve the optimal
solution of the nonlinear flow system. However, it always needs more memory than the other embedding models. If there is not enough memory, the El fully linear embedding model or the RM response matrix model needs the least memory.
References


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Table 1. Summary of Solution Procedures and Formulas for Alternative Models

<table>
<thead>
<tr>
<th>Original Eq. /Models</th>
<th>Transmissivity</th>
<th>External flows</th>
</tr>
</thead>
<tbody>
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<td></td>
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<td>Unconfined</td>
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<tr>
<td>Original Eq.</td>
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<td>Nonlinear</td>
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<tr>
<td>E1</td>
<td>Constant</td>
<td>LP&amp;Cycle (^b)</td>
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<tr>
<td>E2</td>
<td>Constant</td>
<td>LP&amp;Cycle (^b)</td>
</tr>
<tr>
<td>E3</td>
<td>Constant</td>
<td>NLP(^c)</td>
</tr>
<tr>
<td>RM</td>
<td>Constant</td>
<td>LP&amp;Cycle (^b)</td>
</tr>
</tbody>
</table>

\(^a\)LP means a linear equation.

\(^b\)LP&Cycle means a linearized equation which requires cycling.

\(^c\)NLP means a nonlinear equation.

\(^d\)DNLP means an equation for nonlinear programming with discontinuous derivatives.
<table>
<thead>
<tr>
<th>Model components</th>
<th>Models</th>
<th>E1</th>
<th>E2</th>
<th>E3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Objective function</td>
<td></td>
<td>Eq.1</td>
<td>Eq.1</td>
<td>Eq.1</td>
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<td></td>
<td>(LP)</td>
<td>(LP)</td>
<td>(LP)</td>
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<td>2. Constraints</td>
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<td>Eq.2</td>
<td>Eq.2</td>
<td>Eq.2</td>
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<td>Flow equation</td>
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<td>(NLP)</td>
<td>(NLP)</td>
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<td>Hydraulic conductances: C and CR</td>
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<td>(C⁺)</td>
<td>(C⁺)</td>
<td>Eqs.3a,3b</td>
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<tr>
<td>Drain discharge</td>
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<td>Eq.5a</td>
<td>Eq.5b</td>
<td>Eq.5b</td>
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<td></td>
<td></td>
<td>(LP)</td>
<td>(DNLP)</td>
<td>(DNLP)</td>
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<td>3. Bounds</td>
<td>Head of the upper layer</td>
<td>H ≥ -150 ft</td>
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<td>Head at the pumping cell</td>
<td>H ≥ 30 ft</td>
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<tr>
<td></td>
<td>Pumping rate</td>
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<td></td>
</tr>
<tr>
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<td>Flux across constant boundary</td>
<td>q₅ ≥ 0.0 q₆ ≥ 0.0</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>Discharge from drain</td>
<td>q₇ ≥ 0.0 q₈ ≥ 0.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4. Variable declaration</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Positive</td>
<td></td>
<td>gp</td>
<td>h,q⁵,q⁶</td>
<td>gp</td>
</tr>
<tr>
<td>Default (free)</td>
<td></td>
<td>h,q⁵,q⁶</td>
<td>h,q⁵,q₆,CC,CR</td>
<td>obj</td>
</tr>
<tr>
<td>Free</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5. MINOS solver</td>
<td></td>
<td>LP</td>
<td>DNLP</td>
<td>DNLP</td>
</tr>
<tr>
<td>6. Cyclic Procedure</td>
<td></td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
</tr>
</tbody>
</table>

*C means constant in a cycle.

*When the DNLP solver is used, appropriate bounds should be specified on every variable.
Table 3. Response Matrix Model

<table>
<thead>
<tr>
<th>Model components</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>A. Pre-ICG</strong></td>
<td>Yes</td>
</tr>
<tr>
<td><strong>B. ICG</strong></td>
<td>Yes</td>
</tr>
<tr>
<td><strong>C. Management model</strong></td>
<td></td>
</tr>
<tr>
<td>1. Objective function</td>
<td>Eq.1 (LP)</td>
</tr>
<tr>
<td>2. Constraints</td>
<td></td>
</tr>
<tr>
<td>Summation for head Eq.13 (LP)</td>
<td></td>
</tr>
<tr>
<td>Hydraulic conductances</td>
<td>(C')</td>
</tr>
<tr>
<td>for VHCf (pumping cell)</td>
<td>Eq.13</td>
</tr>
<tr>
<td>Flux across constant head boundary (q')</td>
<td>Post-optimization(^b)</td>
</tr>
<tr>
<td>Drain discharge (q')</td>
<td>Post-optimization(^b)</td>
</tr>
<tr>
<td>3. Bounds</td>
<td></td>
</tr>
<tr>
<td>Head of the upper layer</td>
<td>(H \geq -150\ ft)</td>
</tr>
<tr>
<td>Head at the pumping cell of the lower layer</td>
<td>(H \geq 30\ ft)</td>
</tr>
<tr>
<td>Pumping rate</td>
<td>(4\ cfs \leq gp \leq 16\ cfs)</td>
</tr>
<tr>
<td>4. Variable declaration</td>
<td></td>
</tr>
<tr>
<td>Positive</td>
<td>gp</td>
</tr>
<tr>
<td>Default (free)</td>
<td>h</td>
</tr>
<tr>
<td>Free</td>
<td>obj</td>
</tr>
<tr>
<td>5. Solver of MINOS</td>
<td>LP</td>
</tr>
<tr>
<td>6. Cyclic Procedure</td>
<td>Yes</td>
</tr>
</tbody>
</table>

\(^c\)C means constant in a cycle.

\(^b\)q' and q' are not formulated as constraints in the management model but are calculated using the Pre-ICG.
### Table 4. Summary of Computational Statistics

<table>
<thead>
<tr>
<th>Item</th>
<th>E1</th>
<th>E2</th>
<th>E3</th>
<th>RM</th>
</tr>
</thead>
<tbody>
<tr>
<td>A. Number of nonzero elements</td>
<td>4158</td>
<td>4156</td>
<td>7585</td>
<td>49</td>
</tr>
<tr>
<td>linear</td>
<td>4158</td>
<td>4156</td>
<td>4606</td>
<td>49</td>
</tr>
<tr>
<td>nonlinear</td>
<td>0</td>
<td>9</td>
<td>2979</td>
<td>0</td>
</tr>
<tr>
<td>B. Number of equations</td>
<td>685</td>
<td>685</td>
<td>1330</td>
<td>7</td>
</tr>
<tr>
<td>C. Number of variables</td>
<td>721</td>
<td>721</td>
<td>1396</td>
<td>13</td>
</tr>
<tr>
<td>D. Memory (Mbytes)</td>
<td>0.40</td>
<td>0.46</td>
<td>1.31</td>
<td></td>
</tr>
<tr>
<td>E. Cycles</td>
<td>6</td>
<td>6</td>
<td>1</td>
<td>6</td>
</tr>
<tr>
<td>F. Total CPU time (min:sec)</td>
<td>3:05</td>
<td>3:50</td>
<td>2:41</td>
<td>5:17</td>
</tr>
<tr>
<td>G. Convergence in the six th cycle</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LDHC(^a) (ft)</td>
<td>&lt; 0.001(^c)</td>
<td>&lt; 0.001(^c)</td>
<td>&lt; 0.001(^c)</td>
<td></td>
</tr>
<tr>
<td>TDHC(^b) (ft)</td>
<td>0.060</td>
<td>0.013</td>
<td>&lt; 0.001(^c)</td>
<td></td>
</tr>
<tr>
<td>H. Largest head difference</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>between E3 and other models</td>
<td>&lt; 0.001(^c)</td>
<td>&lt; 0.001(^c)</td>
<td>&lt; 0.001(^c)</td>
<td></td>
</tr>
</tbody>
</table>

\(^a\)LDHC is the largest absolute difference between heads for two consecutive cycles.

\(^b\)TDHC is the total absolute difference between heads for two consecutive cycles. E1, E2, and E3 estimate heads at 625 cells. RM estimates heads at 6 cells.

\(^c\)< 0.001 is less than 0.001.

\(^d\)E3 computes the optimal strategy at the first optimization. No cycling is needed.
<table>
<thead>
<tr>
<th>Alternatives</th>
<th>$N_{Z_t} = N_{Z_0} + \text{increments}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Embedding Method models</strong></td>
<td></td>
</tr>
<tr>
<td>E1</td>
<td>$4146 + 2N_{P_t}$</td>
</tr>
<tr>
<td>E2</td>
<td>$4153 + 2N_{P_t}$</td>
</tr>
<tr>
<td>E3</td>
<td>$7573 + 2N_{P_t}$</td>
</tr>
<tr>
<td><strong>Response Matrix Approach model</strong></td>
<td></td>
</tr>
<tr>
<td>RM</td>
<td>$1 + 0.5N_{P_t} {(6 + (N_{P_t} - 1)\times 2)}$</td>
</tr>
</tbody>
</table>

$N_{Z_t}$ = total number of non-zero elements.

$N_{P_t}$ = total number of pumping well cells.

$N_{Z_0}$ = number of nonzero elements with no pumping cells.
Fig. 1. Flow charts of solving procedure for the embedding models.
Fig. 2  Summary of solution procedures for the original and modified McDonald and Harbaugh models.
Fig. 3  Flow chart of solution procedure for the response matrix model.
Fig. 4. Hypothetical three-layer aquifer system.
**LEGEND**

- **Variable head cell**
- **Variable head cell with pumping**

<table>
<thead>
<tr>
<th>Pumping well</th>
<th>Discharge (cfs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GP1</td>
<td>9.396</td>
</tr>
<tr>
<td>GP2</td>
<td>11.294</td>
</tr>
<tr>
<td>GP3</td>
<td>10.368</td>
</tr>
<tr>
<td>GP4</td>
<td>10.868</td>
</tr>
<tr>
<td>GP5</td>
<td>13.842</td>
</tr>
<tr>
<td>GP6</td>
<td>13.267</td>
</tr>
</tbody>
</table>

**Fig. 5.** Potentiometric heads in Layer 3 (the lower layer).