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A COUPLED SIMULATION-OPTIMIZATION TECHNIQUE FOR PROTECTING MUNICIPAL GROUND-WATER SUPPLIES FROM CONTAMINATION

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Abstract

A technique based on numerical ground-water flow modeling and unconstrained nonlinear optimization has been developed to provide guidance for protecting municipal ground-water supplies from contamination through capture zone management. The technique involves conventional finite-difference ground-water flow modeling and numerical flowpath/travel time calculation coupled with nonlinear mathematical programming. The objective of the technique is to specify pumping rates for wells in a wellfield such that the configuration of capture zones in relation to existing potential sources of contamination minimizes the risk of contamination while maintaining the required total water output from the wellfield. An important feature of the technique is its ability to incorporate realistic boundary conditions, complicated aquifer configurations, and spatially varying aquifer properties to whatever degree site-specific data are available. Also, the technique is implemented on a personal computer. This approach to ground water supply protection has an obvious advantage over conventional wellhead protection area delineation in that a greater level of protection can be achieved if potential contaminant sources are not even included in capture zones, rather than attempting to reduce the threat of those sources. A hypothetical aquifer system with spatially varying properties was used to demonstrate and verify the effectiveness of the technique. Also, work is currently underway to apply the technique to a real wellfield in Pekin, Illinois. These efforts demonstrate the utility of an innovative modeling technique in ground water quality protection.

Introduction

The protection of municipal ground-water supplies from contamination has received considerable attention recently due to the 1986 amendments to the Safe Drinking Water Act (SDWA) which require the establishment of State Wellhead Protection Programs. A key element of wellhead protection under the SDWA is the determination of zones, called wellhead protection areas (WHPAs), within which contaminant source assessment and management will be addressed. The U. S. Environmental Protection Agency (USEPA) defines a WHPA as "the surface and subsurface area surrounding a water well or wellfield, supplying a public water system, through which contaminants are reasonably likely to move

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toward and reach such well or wellfield." (USEPA, 1987). A variety of techniques have been suggested for delineating WHPAs, ranging in complexity from the specification of fixed radii circles around a well to the implementation of numerical models to define the contributing area, or capture zone, of a well or wellfield. The USEPA (1987) recommends basing WHPAs on time-specific contributing areas to wells, which are based on the steady-state ground-water time of travel to a well.

WHPAs based on time-related capture zones are typically determined using current or average operating characteristics (pumping) of a well or wellfield. Therefore, the capture zone and corresponding WHPA has been viewed as a static property of a particular well or wellfield. Determining such a zone and then instituting contaminant source assessment and land use restrictions within the WHPA is certainly a viable approach to reducing the risk of contamination of municipal ground-water supplies. However, where pre-existing, potentially contaminating land uses may exist within the capture zones of the wells, a greater risk reduction can be achieved if the configurations of the capture zones (in relation to existing threatening land uses) are changed, via a different pumping scheme, to minimize the number of potential contaminant sources included in the capture zones. It is undoubtedly more favorable (in terms of minimizing contamination risk) if a capture zone for a well does not include a particular source rather than attempting to reduce the threat of the source. Some existing land-uses (e.g., landfills) may always present a threat, even if the site has been remediated to the greatest extent possible.

In general, the size of the time-specific capture zone for a particular well increases as more water is pumped from the well. Increasing the area of a capture zone will in many cases increase the risk that the well may become contaminated simply because more potential contaminant sources may be included in the capture zone. By the same argument, reducing the pumping of a well will in many cases reduce the risk of contamination. In this case, managing the extent of the capture zone in relation to potential sources requires a trade-off. If risk (measured by the number of potential contaminant sources located inside the capture zone) is to be reduced, total water production from the well must also be reduced which means that water demands may go unmet. The ground-water protection strategy introduced in this paper is based on the idea that it may be possible to compensate for this unmet demand by increasing the pumping of another well if the other well is located such that additional pumping would not increase (and possibly decrease via well interference) the number of potential sources in the capture zone.

If a ground water supply system simply consists of two independent wells, specification of new pumping rates to minimize risk would follow simple guidelines: decrease pumping where there is high risk, and increase pumping where the risk is low. Within a wellfield, however, the hydraulic interactions between the wells are complex, and the relationships between pumpage of individual wells and total risk to the water supply is less obvious. When several wells are involved, changing the pumping of one well may significantly alter the capture zones (and therefore the risk of contamination) of other wells in the wellfield, even if the pumping rates of the other wells were unchanged. An example of such a situation was illustrated by Wehrmann and Varljen (1990). Furthermore, with several wells, compensation for a decrease in pumping of one well can be attained in a variety of different ways (each one possibly presenting different risk levels), as opposed to a two-well system where every decrease in withdrawl from one well can only be compensated by an equal withdrawl from the other well. Therefore, for a wellfield, there is a need for the development of a coupled simulation-optimization approach to determine optimum pumping rates that would result in the minimum number of potential sources included in the capture zones while meeting the withdrawl requirements .

This paper presents a simulation-optimization approach that may be used for determining optimum pumping rates. The approach ensures that the optimized pumping rates will achieve the greatest risk reduction possible (by minimizing the number of potential contaminant sources included in the capture zones) while maintaining the required water output from the wellfield. Also presented is a demonstration of the technique and an exercise aimed at verifying the optimality of the pumping rates.

Approach

Problem Formulation

The use of predictive ground-water modeling, which is required for the delineation of time-related capture-zones, makes it possible to simulate the effects of different pumping scenarios on the extent and configuration of these zones. As valuable as this simulation capability is, it can only predict the outcome of a given pumping scheme. It cannot directly find the "best" scheme by itself. It would be possible, of course, to operate the simulation model for a wide range of pumping schemes and then select the best alternative in terms of the objectives (i.e., minimizing risk) and constraints (maintaining output). Use of such an approach however sidesteps rigorous formulation (there is no guarantee that the "best" pumping scheme will be found) and fails to consider important physical and operational restrictions, not to mention the fact that it has the potential to become extremely time consuming because of the large number of simulations that would be needed. What is required to determine optimum pumping rates is not a simulation model alone, but a simulation model combined with an optimization model. A combined model considers the particular behavior of a given ground-water system and determines the best, or optimum, operating policy under the necessary objectives and restrictions (i.e., for this example, minimize risk without letting total ground-water withdrawal fall below a specified level). For optimal wellfield management, the combined model is based on the following optimization problem:

$$\begin{aligned} &\text{minimize: } f(q) \\ &\text{subject to: } h(q) = 0 \end{aligned} \tag{1}$$

where

$$f(q) = \sum_{j=1}^{ns} u_j$$

and

$$h(q) = Q - \sum_{i=1}^{nw} q_i$$

where u_j = 1 if source s_j is in the capture zone, or
u_j = 0 if source s_j is not in the capture zone,
ns = number of potential contaminant sources (j),
nw = number of wells in wellfield (i),
Q = target wellfield withdrawal, and
q_i = withdrawal of well i.

This optimization problem may be addressed with an iterative technique. The components and interrelationships of this technique are schematically shown in figure 1. The value of u_j is determined by first simulating ground-water flow, delineating time-related capture zones, and then determining whether or not a potential source, s_j, is included in a capture zone. The u_j's are passed to the optimization algorithm which uses this information to specify new pumping rates, q_i, which are sent back to the simulation model. This procedure continues until the optimum solution is obtained.

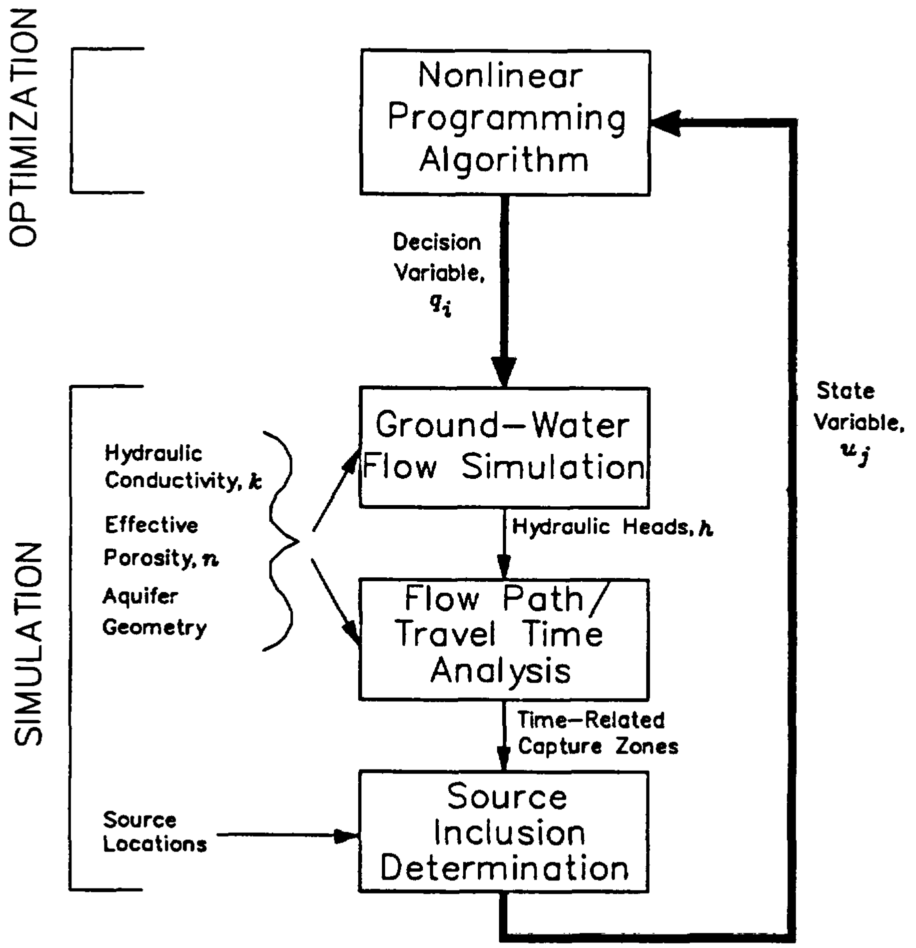

Figure 1. Components and Interrelationships of the Coupled Simulation-Optimization Technique for Wellfield Management.

Problem Solution

Under this coupled simulation-optimization methodology, the ground water system behavior could be simulated using any ground-water flow modeling technique, depending on site conditions and data availability. The complexities of the hydraulics of a wellfield require, however, that the method be capable of considering the interactions of the individual wells in a wellfield. Therefore, a two-dimensional, steady state finite-difference technique was selected. This technique also allows the incorporation of spatially-varying aquifer properties if adequate data are available. The specific formulation used in the coupled simulation-optimization code utilizes a direct matrix solution technique (Cholesky decomposition) with back substitution for efficiency. This way, the coefficient matrix of the set of simultaneous equations only has to be decomposed once when the problem is initiated instead of repeatedly for each iteration of the optimization process. Data requirements for this step include pumping rates, aquifer geometry (aerial extent and thickness), boundary conditions, and hydraulic conductivity values. It must be pointed out that this step is quite critical in this coupled simulation-optimization methodology. Therefore, all standard guidelines for ground water modeling (such as those presented by Mercer and Faust, 1981) covering all aspects of the modeling process (e.g., grid construction, calibration, etc.) must be strictly followed.

Capture zone determination was accomplished using a reverse pathline analysis technique based on that of Shafer (1987a). For inclusion in the simulation-optimization technique, the capture zone calculation was modified to allow fewer pathlines to be used when there is a steep regional gradient. In such situations, reverse pathlines emanating from the well in the downgradient direction curl around in the regional flow field and end upgradient from the well. Therefore, the conventional capture zone delineation technique requires a very large number of pathlines to define the capture zone in the downgradient direction. Because the simulation-optimization methodology is an iterative approach, a great improvement in efficiency can be achieved if fewer pathlines are required for capture zone delineation. Therefore, instead of calculating a large number of reverse pathlines, the outermost paths were used to estimate the extent of the capture zone downgradient from the well (pathline endpoints were still used in the upgradient direction). Several comparisons of capture zones estimated with this technique with those calculated based on a very large number of reverse paths determined with the code GWPATH (Shafer, 1987b) indicate that no significant error is introduced by this approximation.

The inclusion of potential contaminant sources in capture zones was determined by first mapping the entire problem to local polar coordinate systems for each well. Radial distances away from pumping wells of potential sources were compared to the radius of the capture zones at the angular coordinate of the potential source. If the radial distance of the potential source was less than the radius of the capture zone, the source was considered to be a risk to the well.

A penalty function approach (Bazaraa and Shetty, 1979) was used to address the optimization component of the problem. Shafer and Vail (1987) applied such an approach to the optimal control of ground-water contaminant plumes. The basis of the penalty function approach is to convert the constrained problem into an equivalent unconstrained problem so that unconstrained optimization methods can be used, thus allowing the decoupling of the simulation component from the optimization component. The constraints of the original problem are placed into the objective function via a penalty parameter in such a way that a penalty is incurred for any violation of the constraints. The objective function has two components: a 'performance' part, $f(q)$, which is what is actually to be minimized, and a 'constraint' part, $h(q)$, which ensures feasibility.

Using this approach, the original optimization problem (i.e., equation 1) is transformed into the following equivalent unconstrained problem:

$$\begin{aligned} &\text{minimize: } f(q) + \beta h(q) \\ &\text{subject to: } q \in E_n \end{aligned} \tag{2}$$

where,

E_n denotes n-dimensional Euclidean space (the collection of all vectors of dimension n), and

β is the penalty parameter.

It can be seen that the optimal solution to the above problem must have $h(q)$ close to zero, because otherwise a large penalty $\beta h(q)$ will be incurred. The optimization is conducted by applying a minimization algorithm to equation (2).

The principal advantage of this methodology is that the simulation component of the methodology is not embedded in the constraint set of the optimization problem. Thus, the ground-water flow simulation algorithm is implemented independently from the minimization algorithm. As indicated by Shafer and Vail (1987), such an indirectly coupled simulation-optimization approach greatly facilitates the evaluation of complex field-scale problems.

This approach is not without limitations, however. For non-convex objective functions, it is possible that multiple solutions could be generated using different initial conditions, therefore there is no guarantee that a globally optimum solution will be found. Also, there are some computational difficulties associated with ill-conditioning. This ill-conditioning can occur if the penalty parameter, β, has not been selected carefully. If β is too large, more emphasis is placed on feasibility, so the minimization algorithm may terminate prematurely as soon as a feasible solution is encountered. Conversely, if the penalty parameter is too small, not enough emphasis will be placed on feasibility and the constraint component of the objective function will be violated. This problem can also occur with certain objective functions, regardless of the value of the penalty parameter. This is likely to happen when the values of the constraint component of the objective function are not directly comparable with those of the performance part. This is the situation that arises with the optimal wellfield management problem. The performance part has a value corresponding to the number of sources included in the capture zones of the wells in the wellfield (typically a relatively low integer). The constraint part of the objective function, however, has values of pumping rates, and therefore may be orders of magnitude greater than the values of the performance part of the objective function. In this situation, a violation of the pumping constraint by 200 gallons per day, for example, could be insignificant, but would easily overshadow the values of the performance component.

This problem was addressed by changing the form of the objective function. First, the performance and constraint parts of the objective function were changed to ratios (sources included to number of sources; total withdrawal to target withdrawal), so that both parts varied between 0 and 1. Secondly, an exponential penalty was added to the constraint part of the objective function so that large violations of the pumping constraint would cause a much larger penalty than small violations. With such an objective function, the emphasis shifts from feasibility to performance when the pumping rates are close to the target. The resulting objective function has the following form:

$$\frac{\sum_{j=1}^{ns} u_j}{ns} + \left[\beta \left| 1 - \frac{\sum_{i=1}^{nw} q_i}{Q} \right| \right]^{1.5} \tag{3}$$

It was immediately recognized that analytical search techniques (those that require that the mathematical structure of *f* and *h* be such that analytical derivatives of the functions can be computed) would be inappropriate to find the minimum of the above function. Therefore, an experimental search algorithm (Powell, 1964) was used. This computational algorithm belongs to the class of unconstrained optimization procedures referred to as "conjugate direction methods," which are known to be efficient methods for finding the minimum of a function of several variables without calculating derivatives (Rao, 1984). The computer code of Powell's algorithm which was incorporated into the optimal wellfield management code was written by the Operations Research Center, University of California, Berkeley.

Demonstration and Verification

The hypothetical ground-water system used for demonstration and verification of the simulation-optimization technique is shown in figure 2. The system is characterized by no-flow boundaries on the top and bottom and constant head boundaries on each side. Head values were specified at the constant head boundaries such that regional flow (gradient=0.002) would be set up from right to left. The hypothetical aquifer has an average thickness of 200 ft. and is characterized by spatially varying hydraulic conductivity. The hydraulic conductivity distribution is based on a lognormally distributed spatially correlated random field with a mean and variance of 1500 gpd/sq.ft. and 350000, respectively. This distribution is depicted by the contours in figure 2. An effective porosity of 25% was assumed throughout the domain. The wellfield consists of three wells, from which a total withdrawal of 2.0 million gallons per day (MGD) is required. There are 20 potential contaminant sources (designated by 'x's' in figure 2) randomly located throughout the domain. To facilitate ground-water flow simulation and capture zone calculation, a 61×41 ($\Delta x = \Delta y = 150$ft) mesh-centered finite difference grid (also shown in figure 2) was superimposed over the domain.

The simulated hydraulic head distribution and capture zone configurations resulting from an initial pumping strategy are shown in figure 3. This pumping strategy achieves the required withdrawal of 2.0 MGD by pumping each of the three wells at approximately the same rate. Under this operating strategy, a total of 13 potential contaminant sources (total NRS=13) are located within the capture zones of the wells. An alternative pumping strategy was developed through application of the coupled simulation-optimization technique and resulted in the hydraulic head distribution and capture zone configurations shown in figure 4. Under this alternative strategy, the required withdrawal of 2.0 MGD is maintained, while the number of potential contaminant sources located inside the capture zones has been reduced from 13 to 7.

This optimum solution was verified by exhaustively operating the simulation model over an extensive range of possible wellfield operating scenarios. Simulations were conducted for all possible pumping combinations that resulted from individually incrementing the pumping of each well (step=0.2 MGD) from 0.2 MGD to 1.2 MGD. The total wellfield pumpage and number of potential contaminant sources included in the capture zones was recorded for each simulation. These data are plotted in figure 5. Each circle in this plot represents a different pumping scenario. The sizes of the circles are proportional to the value of the objective function (equation 3) for each scenario. It can be seen that several scenarios, each resulting in a different number of sources included, satisfy the pumpage requirement of 2.0 MGD. The optimum solution, of course, is the one that meets this pumpage requirement with the fewest number of sources included in the capture zones. Note that this scenario is depicted by the smallest circle in figure 5, indicating a minimum value of the objective function. As can be seen in figure 5, the optimum scenario will be one that produces 2 MGD and includes 7 potential sources. This exercise serves to verify the optimization procedure in that the optimum solution depicted in figure 5 (total NRS=7) corresponds to the solution shown in figure 4 which was determined independently by the coupled simulation-optimization procedure.

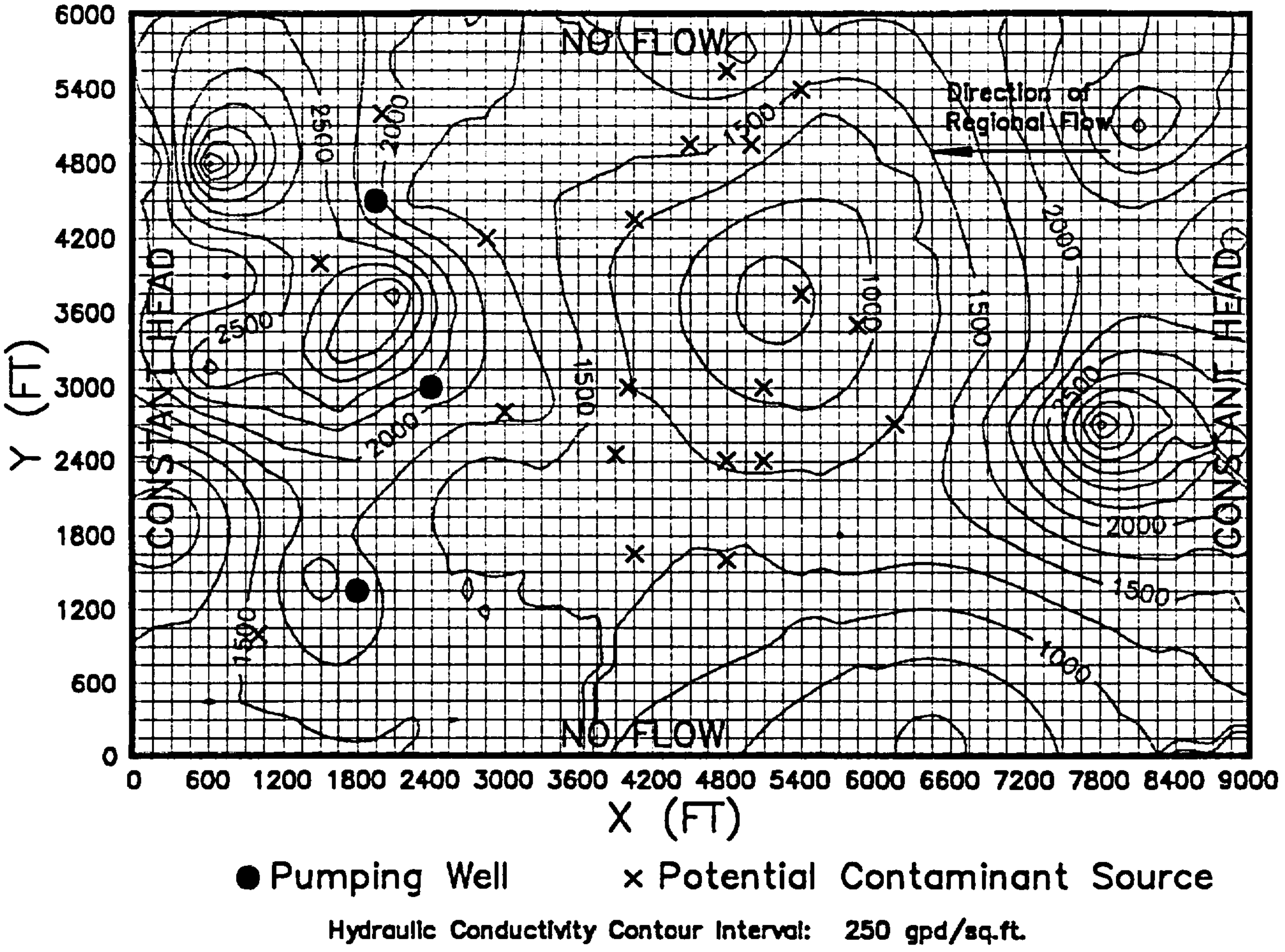

Figure 2. Hypothetical Ground-Water System, Showing Boundary Conditions, Hydraulic Conductivity Distribution, and the Location of Pumping Wells and Potential Contaminant Sources.

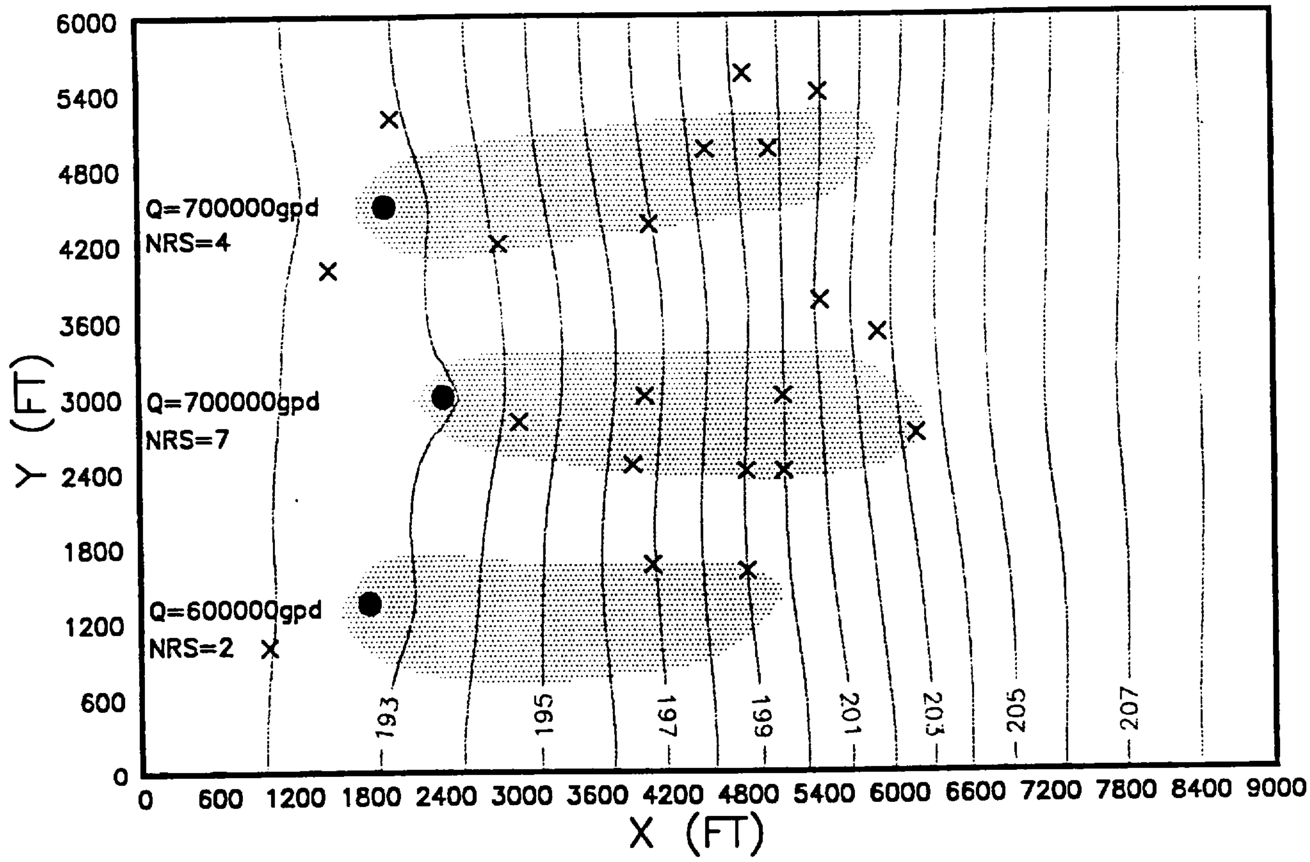

Figure 3. Head Distribution and Capture Zone Configuration Resulting From Initial Pumping Rates

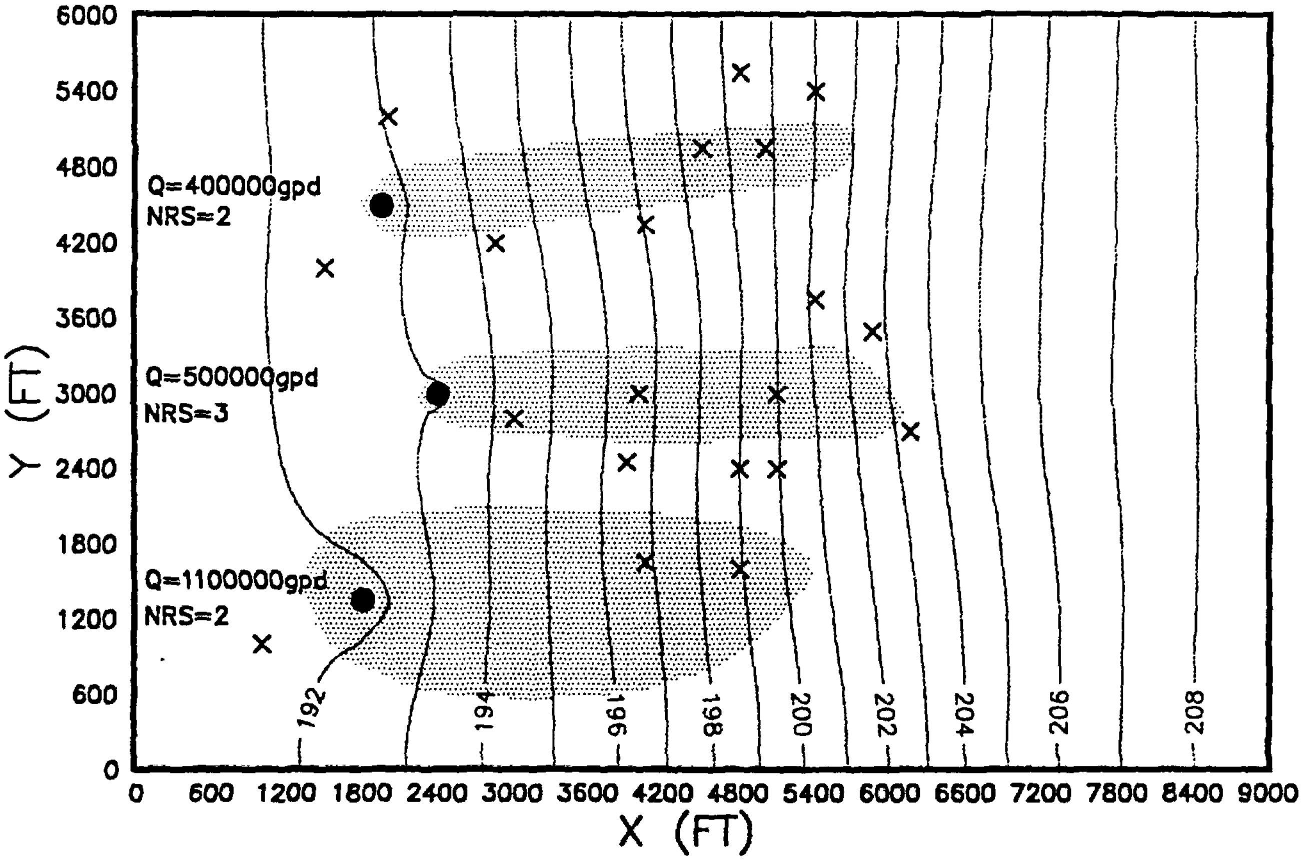

Figure 4. Head Distribution and Capture Zone Configuration Resulting From Optimum Pumping Rates

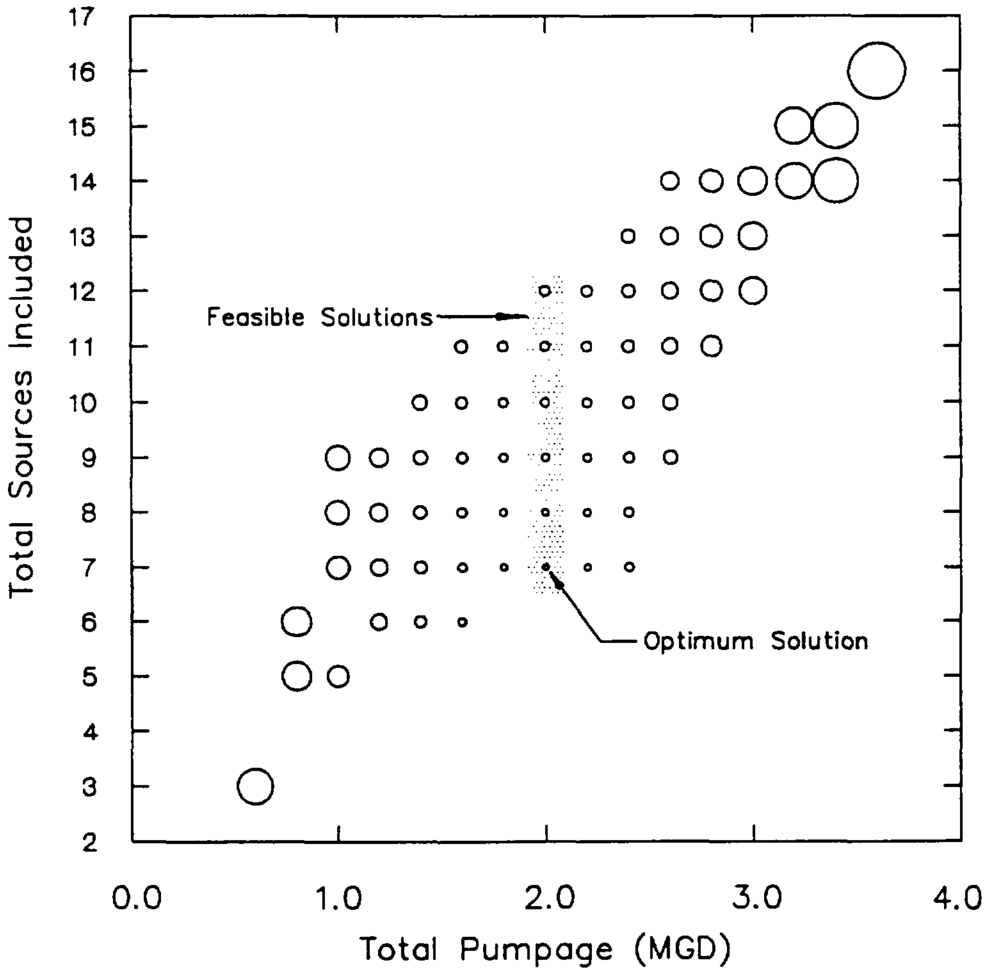

Figure 5. Plot of Sources Included vs Total Pumpage for a Variety of Pumping Scenarios. (size of circle is proportional to value of objective function)

Future Work/Extensions

Now that a computer code has been developed to implement the coupled simulation-optimization technique, it will be useful to assess practical issues associated with the application of such a technique. For this reason the Illinois State Water Survey has begun site characterization and preliminary modeling activities for the wellfield operated by the Illinois American Water Company in Pekin, Illinois. This wellfield contains seven high yield wells that supply approximately 4.5 MGD to the city of Pekin. All of the wells are completed in the very permeable and vulnerable Sankoty Aquifer and are located in a well-developed urban area with several potential sources of contamination located within the capture zones of the wells. At least two of the wells have had a history of contamination. Necessary field data are being collected from the Pekin site so that the ground water flow model can be constructed and calibrated. Potential contaminant source locations are being determined through aerial photograph interpretation and street reconnaissance. The optimization technique will be applied to determine optimum pumping rates after the flow model has been completed.

One other area where additional work is being conducted is in the incorporation of variable risk levels for the potential contaminant sources to be considered by the coupled simulation-optimization model. At this point, the risk of including each source in a capture zone is considered to be equal. This, of course, is a simplification. There is no doubt that some potential sources pose a greater threat than others. This shortcoming can be addressed by adding a 'risk factor coefficient' to the source inclusion part of the objective function. Although this coefficient would have to be subjectively determined on an arbitrary scale, it would greatly enhance the ability of the method to incorporate realistic conditions. Future work will focus on incorporating this coefficient into the objective function and demonstrating how it can enhance the results.

A final area where this method may be enhanced is the incorporation of uncertainty in the estimation of capture zones into the optimization technique. The current optimization technique is based on a deterministic capture zone delineation. Varljen and Shafer (1991) demonstrated that capture zone estimates can be quite uncertain even when data are plentiful. Although a stochastic optimization for this problem approach promises to be a computational challenge, it appears that this should be the next step in the advancement of this management technique.

Conclusions

A technique that can provide guidance for specifying wellfield pumping rates that minimize contamination risk has been presented, demonstrated, and verified. The computer code developed for this application may be implemented on a personal computer with data and operational requirements similar to those for traditional ground-water flow simulation codes. Although practical uncertainties in both the simulation (arising from model parameter uncertainties) and optimization (arising from the complicated form of the objective function) components of the technique make it impossible to guarantee that a unique optimum solution will be found, the technique is certainly valid as a management tool for improving pumping strategies.

NOTE:

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