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COMPUTATIONAL ASPECTS OF CHANCE-CONSTRAINED REGIONAL MODELING

by

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SUMMARY: A methodology that incorporates the stochasticity of an aquifer parameter in a chance-constrained steady-state groundwater management model is presented. Results and computational aspects of the modeling effort are discussed.

KEYWORDS: Modeling, Chance-constraints, Groundwater, Stochasticity, Management, Optimization

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INTRODUCTION

In the past, there has been considerable reluctance on the part of planners and design engineers to use stochastic methods in groundwater management models. However, the presence of uncertainties in estimating aquifer parameters has long been recognized. Fortunately, there have been recent developments in stochastic subsurface flow theory and its practical applications (Gelhar, 1986 and Tung, 1986). Thus, the current trend is to include the natural heterogeneity of aquifers in the governing flow equation by probabilistic in addition to deterministic approaches.

This paper presents a methodology that explicitly incorporates the stochasticity of an aquifer parameter in a chance-constrained formulation of a steady-state groundwater model. The methodology falls under the broad category of explicitly stochastic optimization. It has two parts: a) regional process identification, and b) chance-constrained optimization. The regional process identification establishes and describes the random nature of the aquifer parameter. This is accomplished by a statistical procedure called block kriging. The statistical information obtained from kriging is then utilized as input to an optimization model. This optimization model includes the finite-difference approximation of the steady-state flow equation expressed in probabilistic terms.

The method is applied to a hypothetical area. Results show the applicability of the methodology. Computational aspects of the methodology are discussed. The practical significance of alternative formulations are also included.

PREVIOUS WORK

The need to systematically relate the hydraulic behavior of groundwater flow systems to the optimal use of water supplies has been done by coupling the physical principles of groundwater flow and optimization theory. The "embedding" approach involves inclusion of flow equations as constraints in an optimization model (e.g., Gorelick, 1983, and Peralta, 1985, among many others).

Representation of the random nature of the system components has been attempted and reported in groundwater literature only recently. The need to represent the random nature of aquifer parameters has been recognized by groundwater researchers. A number of methods have been proposed in water resources literature. However, researchers have yet to agree on which method is best (Carrera and Neuman, 1986). Finding the proper representation of the random process has been posed as an identification problem. It involves finding the solution of the inverse problem. Numerous approaches to the inverse problem have been proposed. Ponzini and Lozej (1982) reported excellent results using a comparison model to compute interblock transmissivities. Dagan (1985) presented a methodology of solving the problem of determining the random distribution of transmissivity through unconditional and conditional probabilities. More recently, Carrera and Neuman (1986) published methods of estimating the parameters of steady and unsteady groundwater flow by a maximum likelihood method. Gutjahr and Gelhar (1981) considered hydraulic conductivity as a spatial variable. They showed that variogram analysis yielded consistent results with analytical approximations such as first-order analysis and covariance differential equations. This is significant because it indirectly underscores the importance of kriging as a method of describing the spatial random nature and distribution of aquifer parameters.

Kriging is in itself a well-established method of estimation of random distributions. Marx and Thompson (1987) provide an excellent and concise discussion of the kriging procedure and its practical applications. The block kriging procedure that results in smaller estimation variance when average values of parameters are of interest is adequately discussed by Burgess and Webster (1980).

Researchers have also scrutinized the randomness of system components other than aquifer parameters. Maddock (1974) presented a methodology for finding strategies or rules for a stream-aquifer system. He assumed that the demand for water is a random event. His work is based on the premise that the water resource system operates under stochastic water needs or demands.

Of the numerous stochastic modeling techniques that are available, chance-constrained programming includes random variation as an integral part of the constraint set of an optimization model. More importantly, specified probability limits on constraint violations may be established. From the modeling perspective, chance-constrained formulations are useful because they properly represent the random components of the system. Moreover, water resource modeling and optimum solution computation is facilitated by the ability to develop the deterministic equivalent of an originally stated chance-constrained problem.

Charnes and Cooper (1963) published the first comprehensive presentation of chance-constrained programming. Since then, the technique has been extensively implemented in surface water system studies. In groundwater literature, Tung (1986) reported the applicability of chance-constrained programming with response function groundwater modeling. He included random aquifer parameters in a compliance constraint to realistically restrain the model's performance in a probabilistic situation.

In summary, stochasticity of system parameters is of increasing importance in groundwater modeling. Furthermore, well-established methods like kriging and chance-constrained formulation are available for adequate representation of groundwater system optimization problems.

THEORY AND MODEL FORMULATION

Governing Equation

Consider a hypothetical area that is underlain by an aquifer with large saturated thickness. Assume that the change in saturated thickness with time is insignificant. Furthermore, assume a spatially unchanging hydraulic conductivity and a spatially random saturated thickness.

The aquifer in the study area is assumed to be completely surrounded by a larger area. Thus the surrounding aquifer is a source of recharge through the boundary cells of the hypothetical area. The sole vertical discharge from the area's internal cells is groundwater pumping through wells. No other hydraulic stimuli or stresses occur at internal cells. All other recharge to or discharge from the system occur at constant head cells along the area's boundary.

The Boussinesq equation and Darcy's law govern the aquifer recharge to or discharge from the study area. The Boussinesq equation is commonly used to describe two-dimensional flow through porous media. The equation is expressed in terms of continuous partial derivatives in Equation 1.

$$\frac{\partial}{\partial x}\left(T\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial y}\left(T\frac{\partial H}{\partial y}\right)-Q=S\frac{\partial H}{\partial t} \qquad \ldots 1$$

where T is the transmissivity of the aquifer material, S is the storage coefficient of the aquifer, H is the head and t is time. Under steady-state conditions the right-hand side of Equation 1 vanishes. The resulting equation describes two-dimensional flow where Q is the net volumetric flow into and out of the aquifer if there is no change in head with time. Equation 1 can be written in a finite-difference form to describe flow in a heterogeneous isotropic aquifer. Using block-centered two-dimensional cells to represent the system, Equation 1 becomes:

$$\begin{aligned}&DTU(i,j)\ H(i+1,j) + DTU(i-1,j)\ H(i-1,j)\\&+ DTR(i,j-1)\ H(i,j-1) + DTR(i,j)\ H(i,j+1)\\&- TT(i,j)\ H(i,j) = GP(i,j) + RCH(i,j)\end{aligned} \qquad \ldots 2$$

where

GP(i,j) is the amount of groundwater pumping in cell (i,j) in units of L**3/T,

RCH(i,j) is the recharge in cell (i,j) in units of L**3/T,

H(i,j) is the potentiometric head in cell (i,j) in units of L, DTR(i,j) is the transmissivity between cell (i,j) and cell (i,j+1) in units of L**2/T,

DTU(i,j) is the transmissivity between cell (i,j) and cell (i+1,j) in units of L**2/T,

and TT(i,j) is defined below.

$$TT(i,j) = DTU(i,j) + DTU(i-1,j) + DTR(i,j) + DTR(i,j-1) \qquad ...3$$

In Equation 2 the convention adopted is for flow to be positive if the flow direction is out of the cell. Flow is negative if the flow direction is into the cell. The DTU and DTR terms in Equation 2 are usually substituted by either the geometric mean or the harmonic mean of the transmissivities of adjacent cells. The choice depends on the expected accuracy of the resulting transmissivities of the midpoint of adjacent cells. Assume that hydraulic conductivity is constant for the whole area of interest. Assume further that the saturated thickness is governed by a random process. With these assumptions, Equation 2 can be rewritten as:

$$\begin{aligned} k/2 * [\ & b(i,j)\ H(i+1,j) + b(i+1,j)\ H(i+1,j) \\ & + b(i-1,j)\ H(i-1,j) + b(i,j)\ H(i-1,j) \\ & + b(i,j-1)\ H(i,j-1) + b(i,j)\ H(i,j-1) \\ & + b(i,j)\ H(i,j+1) + b(i,j+1)\ H(i,j+1) \\ & - 4* b(i,j)\ H(i,j) - b(i+1,j)\ H(i,j) \\ & - b(i-1,j)\ H(i,j) - b(i,j+1)\ H(i,j) \\ & - b(i,j-1)\ H(i,j)\ ] = GP(i,j) + RCH(i,j) \qquad ..4 \end{aligned}$$

where k is the hydraulic conductivity that is assumed constant in units of L/T,

b(i,j) is the saturated thickness that is governed by a random process in units of L.

Equation 4 is derived from Equation 2 under the simplifying assumption that the transmissivity between two adjacent cells can be adequately represented by the simple average of the cells' block-centered transmissivities. This assumption is necessary to maintain linear terms on the left hand side of the equation. It is also consistent with the independent random distribution nature of the process that describes the saturated thickness of the aquifer. Thus, the absence of spatial correlation is also implied by arithmetic averaging. One should note that arithmetic averaging is appropriate for internal cells but not for cells adjacent to impermeable boundaries.

To facilitate discussion, Equation 4 is rewritten in the following compact form:

$$k/2 * \sum \underline{b}(i,j)\ \underline{H}(i,j) = GP(i,j) + RCH(i,j) \qquad \ldots 5$$

where the left-hand side of Equation 5 is just an alternative notation for the sum of the terms on the left-hand side of Equation 4.

Probabilistic Constraint and Its Deterministic Equivalent

The net discharge of any cell (i,j) in the aquifer system equals the sum of groundwater pumping and recharge in that cell. In a groundwater management system, each cell also has an associated water need or water demand value. In a management scenario in which available water is insufficient to satisfy potential water demand in each cell, a critical value expressed as a fraction of the water need can be established. Furthermore, the probability that the allowable net discharge and/or recharge in each cell does not exceed the critical value can be defined at a prespecified level of certainty. Thus, the flow equation is used in a chance-contraint expression as:

$$P\{\ k/2 * \sum \underline{b}(i,j)\ \underline{H}(i,j) \leq CR(i,j)\ \} \geq 1 - \alpha \qquad \ldots 6$$

Equation 6 imposes the probability that the net discharge from each cell is less than a prespecified critical value, CR(i,j), is greater than (1 - α). Assuming that the saturated thickness, b(i,j), is sufficiently described by a normally distributed process, with mean m(i,j) and variance var(i,j), the probabilistic constraint (Equation 6) can be rewritten as:

$$k/2*[\ \sum \underline{m}(i,j)\ \underline{H}(i,j) + F^{-1}(\alpha)\ (\ \sum \underline{var}(i,j)\ \underline{H}^{2}(i,j))**0.5] \leq CR(i,j) \qquad ...7$$

where $F^{-1}(\alpha)$ denotes a standard normal deviate corresponding to the normal cumulative distribution function of α. (Stability aspects as a consequence of the conversion from Equation 6 to Equation 7 are mathematically analyzed by Dupacova (1984).) All other notations are consistent with those of Equation 6. For the stated assumptions, the deterministic constraint (Equation 7) can replace the probabilistic constraint (Equation 6).

Problem Formulation

Consider a steady-state management problem where the objective is to maximize total groundwater pumping while satisfying constraints on heads, recharges, and pumping. The amount of groundwater pumping in each cell is also required to be less than the cell's water demand. In addition, the probability that net discharge in each cell does not exceed prespecified critical values is set to $(1 - \alpha)$. This problem is applicable to the scenario described below.

A planning agency for a developing country wishes to compute an optimal sustained groundwater yield pumping strategy for an area. The area is to be an important region for irrigated agricultural production. Naturally, the agency wishes to maximize sustainable groundwater pumping. The agency also recognizes that knowledge of spatially variable saturated thickness is uncertain. Furthermore, agricultural reform policies make the agency desire to spread irrigated acreage out in the area, rather than concentrate it in a few cells.

The agency could simply run max pumping strategies subject to chance-constraints on drawdown, and absolute upper and lower limits on pumping. Setting a lower limit of zero pumping is always easy. Setting a higher value for a lower limit may be infeasible if the aquifer cannot provide enough water. Setting firm upper limits is easy and will not adversely affect identifying feasible solutions. However, as stated, the agency wants to achieve a somewhat egalitarian distribution of pumping. Attempting to achieve arbitrary equality of water rights in a spatially variable system may be hydrologically very unsound (Peralta et al., 1985). Therefore, the agency may wish to use chance-constrained upper bounds on pumping to achieve desired spatial flexibility in developing an optimal strategy. Decision makers (DMs) in this study chose to develop a range of maximum pumping strategies. Each strategy is subject to the constraint that the DMs are x% sure that allocated sustainable pumping in each cell does not exceed certain prespecified values. The confidence level is varied systematically. This approach incorporates uncertain knowledge of aquifer saturated thickness in the upper bound on groundwater pumping allocation.

The problem is mathematically formulated as:

$$\text{Maximize} \quad \sum_{i \in I} \quad \sum_{j \in J} \quad GP(i,j) \qquad \ldots 8$$

subject to:

$$HMIN(i,j) \leq H(i,j) \leq HMAX(i,j) \quad \text{for } i \in I,\ j \in J \qquad \ldots 9$$

$$RCHMIN(i,j) \leq RCH(i,j) \leq RCHMAX(i,j) \quad \text{for } i \in I,\ j \in J \qquad ..10$$

$$GPMIN(i,j) \leq GP(i,j) \leq GPMAX(i,j) \quad \text{for } i \in I,\ j \in J \qquad ..11$$

$$GP(i,j) \leq WAD(i,j) \quad \text{for } i \in I,\ j \in J \qquad ..12$$

and the probability constraint in Equation 6.

Where

HMIN(i,j) is a known lower limit on the potentiometric head in cell (i,j) in units of L,

HMAX(i,j) is a known upper limit on the potentiometric head in cell (i,j) in units of L,

RCHMIN(i,j) is a known lower limit on recharge in cell (i,j) in units of L**3/T,

RCHMAX(i,j) is a known upper limit on recharge in cell (i,j) in units of L**3/T,

GPMIN(i,j) is a known lower limit on groundwater pumping in cell (i,j) in units of L***3/T,

GPMAX(i,j) is a known upper limit on groundwater pumping in cell (i,j) in units of L**3/T,

and WAD(i,j) is the known water need or water demand quantity in units of L**3/T.

All other notations have been defined previously. Equations 8, 9, 10, 11, 12, and 6 consist of a chance-constrained problem where the decision variables are GP(i,j), RCH(i,j) and H(i,j), that is, groundwater pumping, recharge, and potentiometric head; respectively. The formulation implies that the distribution process that governs the random aquifer parameter (in this paper, the saturated thickness) is also known. Assuming that this is the case and that the distribution is normal or can be converted to a normal distribution, Equation 7 can substitute for Equation 6.

The programming problem that includes Equations 8, 9, 10, 11, 12, and 7 (Model A) is a nonlinear programming problem due to the nonlinear terms introduced by Equation 7. Nonlinear programming algorithms are currently available to solve programming problems of this structure. The GAMS/MINOS software package was selected for this paper. It consists of a General Algebraic Modeling System (GAMS) developed by the World Bank (Kendrick and Meeraus, 1985) and a Modular In-Core Nonlinear Optimization System (Murtagh and Saunders, 1983).

NUMERICAL EXPERIMENTS

The formulated problem has been applied to a hypothetical area (Figure 1). The same area was used previously by Peralta and Kowalski (1986). The area consists of 65 cells, 40 of which are internal cells. Head is constant in all peripheral cells. A spatially constant hydraulic conductivity value of 82 m/day (270 ft/day) is assumed. The hypothetical area is a small portion of the Bayou Bartholomew Basin in Arkansas, shown as the irregularly shaped area in Figure 2. The relative position of the hypothetical area is shown as area XYZD in Figure 2.

A standard block kriging procedure was implemented to compute the statistical properties of the random distribution that governs the saturated thickness in the study area. Comparative results of the kriging study are shown in Table I. Results show that the larger the area the greater the variance calculated by block kriging. Results for area ABCD (see Figure 2) differs from that of area EFGH by about 50%. Note that area ABCD includes cells that are outside the basin. Results show that smaller variance and smaller mean estimate are obtained when the rectangular area used in kriging includes cells within the basin. Block kriging estimates are applicable to the center of rectangular study area. More accurate results are possible when block kriging is applied to each of the cells of the hypothetical area. Block kriging done on a cell by cell basis is essentially equivalent to application of punctual kriging. This implies spatial independence of the distribution of the random process of the aquifer parameter for each cell. When a regionalized mean and variance of the aquifer parameter for the entire study area can be justified, block kriging defines the random process just as well as punctual kriging.

Optimal solutions for Model A as formulated above have been systematically calculated for different confidence levels, specified as $(1 - \alpha)$. Critical values in the deterministic equivalent of the chance-constraint are also varied to provide a comparative study of the methodology's application. In the numerical experiments, the critical value CR(i,j) is computed as a fraction (FRAC) of the cell's water demand volume. Table II shows results from two groups of computer runs. These are results when a) FRAC = 0.5, and b) FRAC = 0.9 at varying levels of confidence. The slight (possibly insignificant) trend observed here is that as the confidence level $(1 - \alpha)$ decreases, total optimal pumping also decreases. On the other hand, one expects the number of cells exceeding CR(i,j) to increase with decreasing ($1 - \alpha$). It is also important to point out that total pumping increased slightly (about 1%) for FRAC=0.9 as opposed to FRAC=0.5. In this case, when constraining the probability that fluxes not exceed a critical value, increasing the critical value causes insignificant increase in total pumping.

Computer runs for the small hypothetical area are accomplished using the University of Arkansas IBM/370 in the CMS environment. A typical run required about 5 seconds of CPU time while using the GAMS 2.04 nonlinear optimization package option. It is important to point out though that providing reasonable initial values for the decision variables results in shorter CPU time. Computer runs may terminate before finding the optimal solution. In these cases, changing the initial values is necessary. There were also cases where supplied initial values resulted in infeasibility. Multiple optimal solutions existed in some cases. Based on these observations, application of the methodology to areas with a large number of cells may pose problems due to system size and nonlinearity of the deterministic equivalent of the chance-constrained formulation.

ALTERNATIVE FORMULATIONS

Although the problem formulated as Model A in this paper may have definite practical importance in situations of water scarcity, two alternative formulations are worthy of mention. Changing Equation 6 to:

$$P\{ k/2 * \sum \underline{b}(i,j)\underline{H}(i,j) \geq CR(i,j) \} \geq 1 - \alpha \qquad ...13$$

is appropriate for an entirely different management problem. This formulation is now labelled as Model B. Model B is more applicable in situations where available resource is not as limiting a factor. The model seeks to guarantee at least the critical amount at a particular level of reliability. However, there is no assurance that all problems of model B structure would result in feasible strategies. As Peralta et al. (1985) determined in developing an egalitarian groundwater allocation strategy for correlative rights doctrine based on historic water use, the system may be physically unable to provide the prespecified critical value due to its hydraulics and physical properties. Another formulation improves this weakness. Permit the critical level in each cell to vary by stating the chance-constraint as:

$$P(k/2 * \sum b(i,j)H(i,j) \geq f(i,j)*WAD(i,j)) \geq 1 - \alpha \quad \ldots 14$$

where f(i,j) is a decision variable. It is the fraction of the water demand that can at least be satisfied at confidence level of (1 - α) at each cell. Equation 14 is a chance-constraint similar in purpose to that described by Peralta et al. (1985). The range of possible values for f(i,j) is:

$$0.0 \leq f(i,j) \leq 1.0 \quad \ldots 15$$

The following constraint is also added:

$$f(i,j) \geq d \quad \ldots 16$$

Equation 16 restricts the cell by cell fractional levels to be greater than a particular dummy variable d. Now, changing the objective function to Equation 17 completes Model C.

$$\text{Maximize} \quad d \quad \ldots 17$$

Model C, a model that consists of Equations 17, 9 through 12, and 14 through 16, is a max min problem. The problem seeks the best possible set of fractional levels that will provide water needs at a prespecified level of certainty.

SUMMARY AND CONCLUSIONS

Results of numerical experiments showed that chance-constrained formulation is possible and useful in developing groundwater sustained yield extraction strategies. Computational aspects of the methodology and its practical implications were also discussed. Alternative formulations for several management scenarios are presented. Applicability of the presented models depends on validity of assumptions. Being able to quantitatively describe the random process is crucial to converting the chance-constraint to its deterministic equivalent.

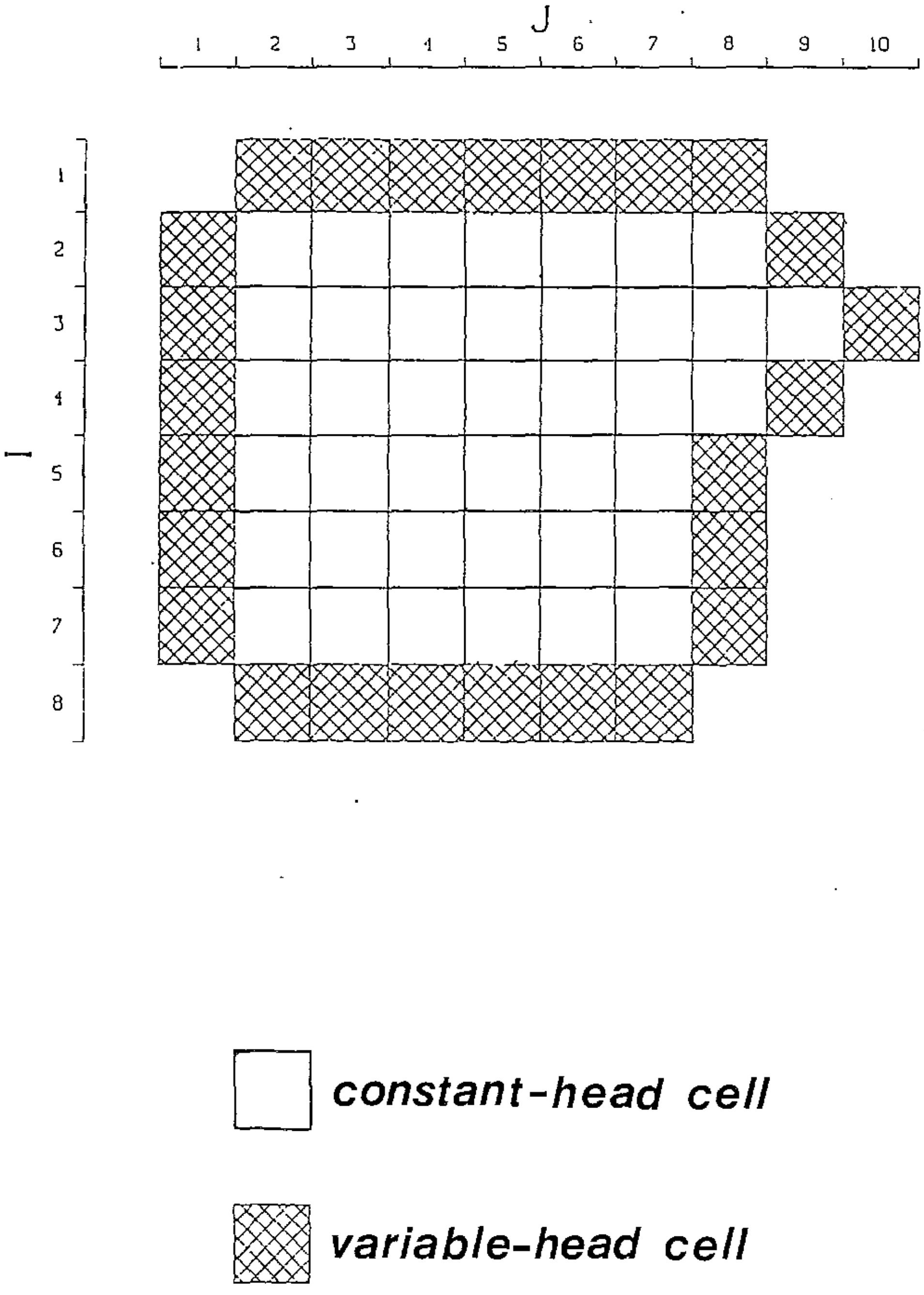

Figure 1. Hypothetical Study Area

AREA SIZE AND BLOCK KRIGING PARAMETERS

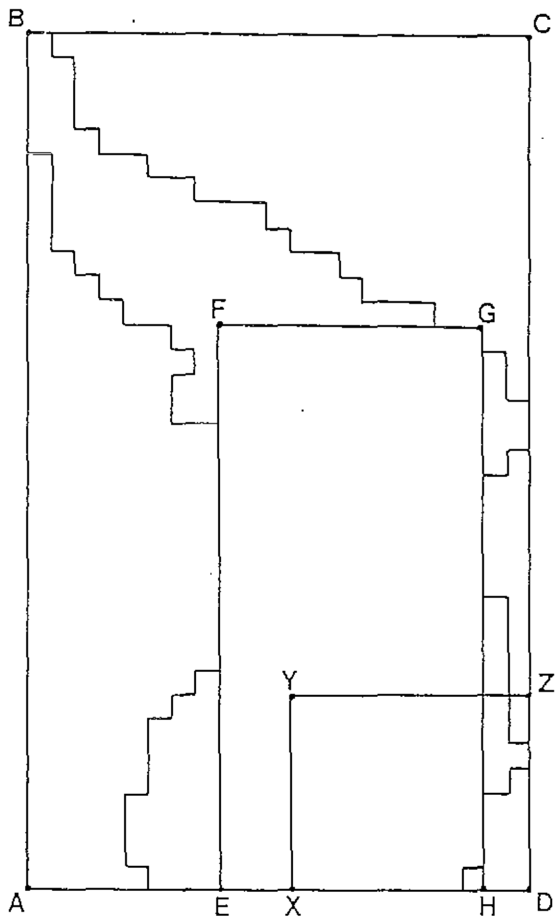

Figure 2. Block Kriging Areas

Table I. Comparison of Block Kriging Results

BLOCK KRIGING RESULTS

AREA	MEAN	STANDARD DEVIATION	INDEX
ABCD	148.03	17.91	3
EFGH	105.62	13.73	3
XYZD	97.91	3.51	19

Table II. Chance-Constrained Modeling Results

COMPARATIVE RESULTS

	FRAC=0.5	FRAC=0.9
$1-\alpha$	OP^*	OP^*
0.95	20.09	21.29
0.90	19.70	20.86
0.80	19.21	20.32
0.60	18.56	19.60

$$OP^* = \frac{\text{OPTIMAL TOTAL GROUNDWATER PUMPING}}{\text{TOTAL WATER NEED}} \times 100$$

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