

Using a hybrid approach to optimize experimental network design for aquifer parameter identification

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Abstract This research develops an optimum design model of groundwater network using genetic algorithm (GA) and modified Newton approach, based on the experimental design conception. The goal of experiment design is to minimize parameter uncertainty, represented by the covariance matrix determinant of estimated parameters. The design problem is constrained by a specified cost and solved by GA and a parameter identification model. The latter estimates optimum parameter value and its associated sensitivity matrices. The general problem is simplified into two classes of network design problems: an observation network design problem and a pumping network design problem. Results explore the relationship

between the experimental design and the physical processes. The proposed model provides an alternative to solve optimization problems for groundwater experimental design.

Keywords Groundwater · Experimental design · Genetic algorithm

Introduction

In environmental monitoring such as groundwater level and quality investigations, the collected data may cause significant uncertainty, including extremely complicated variations in the observed values of measurable characteristics in space and time. Development of efficient procedures for designing and adjusting information-effective monitoring networks is an essential task for more accurately understanding the aquifer property. Therefore, these networks can be used to detect the aquifer property or to characterize groundwater resources for the management.

Evaluation of aquifer parameters (i.e., transmissivity and storage) has been a continuing field of research. Aquifer parameters varying with space are not easily identified. Experimental design is defined as the process of ensuring that a model provides good representation of a real system and identifies the aquifer parameters (Yeh 1986; Heidari and Ranjithan 1998; Hsu

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and Yeh 1989; Nishikawa and Yeh 1989; Carrera et al. 2005). That is, experimental design refers to the process of gathering information from measurements of what is modeled. Experimental conditions for design include the number and locations of pumping and observation wells, and observation frequency and duration (Hsu and Yeh 1989; Nishikawa and Yeh 1989). Systematically optimizing the design involves maximizing parameter estimate reliability, while minimizing experimental design cost is an important consideration. Hsu and Yeh (1989) formulated an experimental design problem as a general mathematical programming problem and demonstrate using a numerical example. They developed a model minimizing experimental design cost whose data yields parameter estimates with required reliability and formulated the experimental design problem as a nonlinear, mixed-integer programming problem. Since the variables are discrete, the gradient-based optimization technique fails. They adopted a heuristic approach to solve a mixed-integer programming problem and a modified Gauss–Newton algorithm to evaluate the design parameters. Nishikawa and Yeh (1989) developed a heuristic algorithm to minimize pumping test cost whose data yields parameter estimates of required reliability. Starting with an initial transmissivity vector, the algorithm sequentially identifies optimal designs, simulates the pumping test, estimates the unknown parameters, and repeats until transmissivity estimates converge. Those studies all formulated the problem as an experimental design problem but only proposed a heuristic method to solve the problem. Since the experimental problem is a nonlinear optimization problem and contains integer variables and a large number of control variables, developing an efficient and systematic algorithm to solve the problem remains a challenging task.

Over the last two decades, optimization techniques, including maximum likelihood method, genetic algorithm, tabu search, and simulated annealing, have been adopted to solve the groundwater problem (Carrera and Neuman 1986; McKinney and Lin 1994; Zheng and Wang 1996; Wang and Zheng 1998; Tung and Chou 2004; Tsai et al. 2003; Tsai and Yeh 2004; Sidiropoulos and Tolikas 2004). Zheng and Wang (1996) applied

two optimization approaches—tabu search and simulated annealing—to identify an optimal parameter structure in a one-dimensional aquifer. McKinney and Lin (1994) used genetic algorithm (GA) to solve groundwater management problems involving operation costs. Results revealed that GA can be used efficiently to solve complex groundwater management problems, as in well field development. Sidiropoulos and Tolikas (2004) used GA to minimize groundwater pumping cost, obtaining optimal well configuration and well discharge. Tsai et al. (2003) and Tsai and Yeh (2004) adopted the hybrid algorithm, which contains a GA, to solve the hierarchical optimization problem. First, GA searches for parameter structural patterns. Then, a quasi-Newton algorithm or Bayesian estimation procedure is used to iteratively improve parameter values. Accordingly, this study applies the GA and modified Gauss–Newton algorithm in the experimental design to solve a discrete, nonlinear, and optimal combinatorial problem. The GA easily determines the dimensions of a well network and the modified Gauss–Newton method estimates parameter values in an experimental design.

This study designs a regional pumping test network that minimizes estimated parameter uncertainty under a given budget. Results demonstrate that GA optimizes well network locations used in automated parameter estimation procedures. Additionally, this work explores the relationship between network location and physical processes.

Mathematical formulation

Experimental network design

This study designs a well network that minimizes estimated parameter uncertainty. Estimated parameter uncertainty is typically related to the covariance matrix:

$$\text{cov}(\hat{T}) \equiv E \left\{ (T - \hat{T})' (T - \hat{T}) \right\} \quad (1)$$

where \hat{T} are the estimated parameters (transmissivity), T are the true parameters, and E represents the mathematical expectation. The

covariance matrix of estimated parameters is approximately (Yeh and Yoon 1981)

$$\text{cov}(\hat{T}) = \frac{F(\hat{T})}{M-L} [J_D^T J_D]^{-1} \tag{2}$$

where

$F(\hat{T})$ the least square error in \hat{T} . A classical criterion for parameter estimation is the least square error. The objective function is defined as $F(\hat{T}) = \text{Min}_T F(T) = [(h(\hat{T}) - h^0)'(h(\hat{T}) - h^0)]$, where $h(\hat{T})$ is the vector of calculated hydraulic head based upon an estimated value of \hat{T} and h^0 is the vector of observed hydraulic head.

- M total number of observations
- L total number of parameters
- J_D Jacobian matrix of h with respect to T , $\left[\frac{\partial h_i}{\partial T_j} \right]_{i=1, \dots, M; j=1, \dots, L}$

The common criteria with least uncertainty for optimal design in groundwater design problems are A-optimality, D-optimality, and E-optimality. A-optimality refers to minimized covariance matrix trace. D-optimality is minimized covariance matrix determinant. E-optimality refers to minimized spectral radius. D-optimality is the most studied of all design criteria (Silvey 1980). The statistical D-optimality criterion for experimental design is herein adopted. The aim of the experimental design problem studied herein is to determine the number and location of observation and pumping wells, so that the design yields the least uncertain parameter estimates using D-optimality. The experimental design problem is formulated as:

$$\text{Min}_{lo, lp, Q(lp)} \left| \text{cov}(\hat{T}) \right| \tag{3}$$

Subject to

$$lo \subset \Omega_o \tag{4a}$$

$$lp \subset \Omega_p \tag{4b}$$

$$\text{num.}(lo) \leq no^{\max} \tag{4c}$$

$$\text{num.}(lp) \leq np^{\max} \tag{4d}$$

$$Q(lp) \leq Q_{\max} \tag{4e}$$

$$F(\hat{T}(lo)) = \text{Min}_T F(T|lo) = \text{Min}_T [(h - h^0)^T (h - h^0) | lo] \tag{4f}$$

$$\frac{\partial}{\partial x} \left(T \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(T \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(T \frac{\partial h}{\partial z} \right) - Q = S \frac{\partial h}{\partial t} \tag{4g}$$

$$d(i, j) \geq \text{dis.}(lo), i \in lo, j \in lo, i \neq j \tag{4h}$$

$$d(i, j) \geq \text{dis.}(lp), i \in lp, j \in lp, i \neq j \tag{4i}$$

where

- $\text{num}(lp)$ number of wells in pumping network
- $\text{num}(lo)$ number of wells in observation network
- lo set of observation network location
- lp set of pumping network location
- Ω_o set of all candidate observation well locations
- Ω_p set of all candidate pumping well locations
- $Q(lp)$ pumping rate at pumping network
- $d(i, j)$ the distance between well i and well j
- no^{\max} maximum number of observation wells
- np^{\max} maximum number of pumping wells
- Q_{\max} maximum pumping rate
- $\text{dis}(lo)$ minimum distance between observation wells
- $\text{dis}(lp)$ minimum distance between pumping wells

Model constraints are given by Eqs. 4a–4i, and with the following meanings: Eqs. 4a and 4b define possible locations for observation and pumping wells in the candidate observation well locations (Ω_o) and pumping well locations (Ω_p). Equations 4c and 4d give the maximum number of observation and pumping wells. Equation 4e limits the pumping rate. Equation 4f estimates parameters by minimizing least square errors. Equation 4g is the groundwater flow equation for the hydraulic head response in an isotropic and confined aquifer using MODFLOW, where h is the hydraulic head; Q is the source/sink term; S is the aquifer storage. The MODFLOW model was initially

documented by McDonald and Harbaugh (1984). The MODFLOW is a physical finite-difference numerical flow model and a computer program developed by the US Geological Survey that numerically solves three-dimensional partial-differential equations for groundwater flow through a porous medium using a finite-difference method (McDonald and Harbaugh 1984; Harbaugh et al. 2000). In addition, Eqs. 4h and 4i are the well distance constraints for considering the well density.

Observation and pumping network design

The general experimental design problem, given by Eqs. 3 and 4a, is split into two sub-problems for simplicity: an observation network design problem and a pumping network design problem.

1. Observation network design

The objective function is defined as

$$\text{Min}_{lo} \left| \text{cov}(\hat{T}) \right| \tag{5}$$

Subject to

$$lo \subset \Omega_o \tag{6a}$$

$$\text{num.}(lo) \leq no^{\text{max}} \tag{6b}$$

$$\begin{aligned} F(\hat{T}(lo)) &= \text{Min}_T F(T|lo) \\ &= \text{Min}_T \left[(h - h^0)^T (h - h^0) | lo \right] \end{aligned} \tag{6c}$$

$$\begin{aligned} \frac{\partial}{\partial x} \left(T \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(T \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(T \frac{\partial h}{\partial z} \right) - Q \\ = S \frac{\partial h}{\partial t} \end{aligned} \tag{6d}$$

$$d(i, j) \geq \text{dis.}(lo), i \in lo, j \in lo, i \neq j \tag{6e}$$

2. Pumping network design

The objective function is defined as

$$\text{Min}_{lp, Q(lp)} \left| \text{cov}(\hat{T}) \right| \tag{7}$$

Subject to

$$lp \subset \Omega_p \tag{8a}$$

$$Q(lp) \leq Q_{\text{max}} \tag{8b}$$

$$\text{num.}(lp) \leq np^{\text{max}} \tag{8c}$$

$$\begin{aligned} F(\hat{T}(lo)) &= \text{Min}_T F(T|lo) \\ &= \text{Min}_T \left[(h - h^0)^T (h - h^0) | lo \right] \end{aligned} \tag{8d}$$

$$\begin{aligned} \frac{\partial}{\partial x} \left(T \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(T \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(T \frac{\partial h}{\partial z} \right) - Q \\ = S \frac{\partial h}{\partial t} \end{aligned} \tag{8e}$$

$$d(i, j) \geq \text{dis.}(lp), i \in lp, j \in lp, i \neq j \tag{8f}$$

GA-based procedure

Problems in the study are mixed-integer nonlinear time-varying problems with discontinuous variables (pumping/observation well locations) and continuous variables (estimated transmissivity), and cannot be solved by a single conventional optimization scheme. Therefore, this study further explores the problem structure and uses the hybrid algorithm to search for (1) where to construct an observation network or a pumping network and (2) estimated parameter values. The GA-based procedure determines the number and locations of observation and pumping wells in GA; then, the parameters are estimated for a given network design using the modified Gauss–Newton method with the least uncertainty. Figure 1 shows the conceptual design algorithm with the experiment design and parameter identification.

Stage A: Encoding

Analogous with biological systems, each chromosome bit is regarded as a gene and the string defines the genetic characteristics of an individual population. Decision variables encode to the binary string. The decision variables of these two problems differ. In problem 1, each chromosome bit represents candidate site location for an observation well. In problem 2, the chromosome bit represents candidate site location for a pumping well. If the value of each chromosome bit equals one, then a well is located at the associated

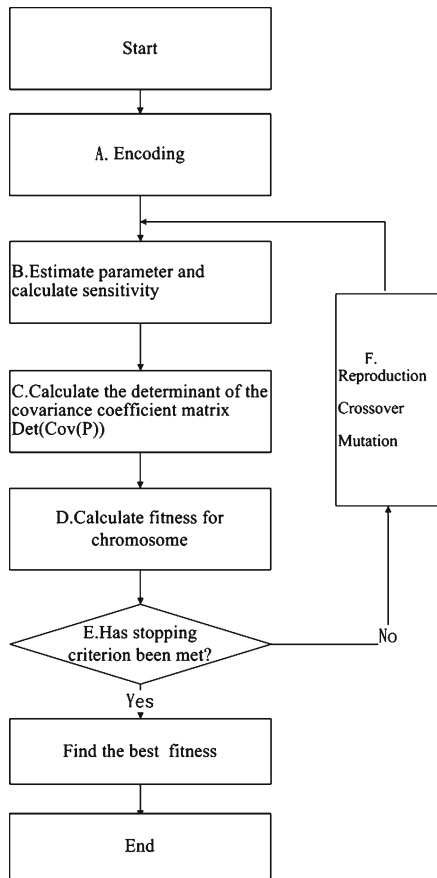


Fig. 1 Flowchart of design algorithm

candidate site. Otherwise, if the value of a bit is zero, then a well will not be installed.

Stage B: Estimate parameters and calculate sensitivity

After encoding the network design, the parameter (transmissivity) is estimated using UCODE (Poeter and Hill 1998). UCODE is a computer code for the universal inverse model. UCODE minimizes a weighted least-squares objective function with respect to parameter values using the modified Gauss–Newton method. This process is called parameter identification and is specified by Eqs. 4f and 4g.

This step determines sensitivity coefficients, which are elements of the Jacobian matrix. Sensitivity is the ratio of head difference to parameter perturbation. Parameter value differs slightly as it is perturbed from its unperturbed value.

Stage C: Calculate the covariance matrix determinant

This step calculates the covariance matrix determinant in Eq. 2.

Stage D: Calculate fitness for each chromosome

This step calculates the fitness of each chromosome. Fitness consists of the objective function and the penalty term if the decision variable is violated by the constraints (Hilton and Culver 2000).

Stage E: Has the stopping criteria been met?

This step checks the stopping criterion, based on the change in objective function and maximum generation. If the best design does not improve over 20 generations or a number of generations correspond to 100 generations, then the algorithm terminates.

Stage F: Reproduction, crossover, and mutation

The GA nucleus involves three operators—the reproduction operator, the crossover operator, and the mutation operator. If the model has not met the stopping criteria, then the parent generation undergoes reproduction, crossover, and mutation, generating the next generation of offspring (Goldberg 1989). The simple approach applying the solution operator, adopted in this

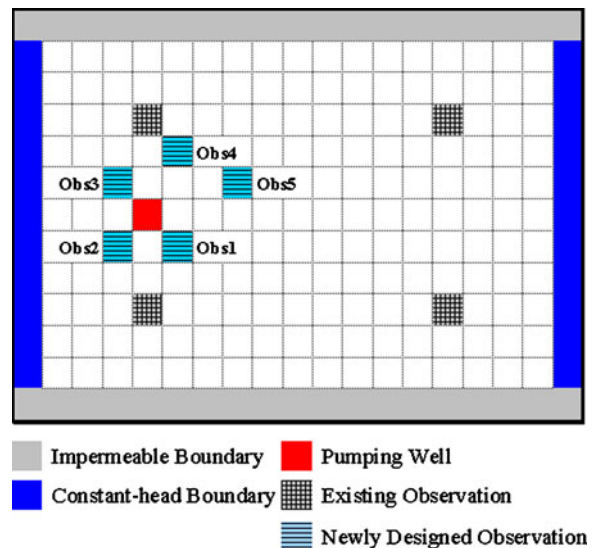


Fig. 2 Results in case 1

Table 1 Location and sensitivity of the additional observation

		Obs1	Obs2	Obs3	Obs4	Obs5
Case 1	Location	(6, 8)	(4, 8)	(4, 6)	(6, 5)	(8, 7)
	Sensitivity (s/m)	55.67	47.00	47.00	45.49	42.38
Case 2	Location	(11, 6)	(11, 8)	(9, 6)	(8, 8)	(13, 7)
	Sensitivity (s/m)	72.57	72.57	72.53	60.15	50.80
Case 3	Location	(14, 8)	(14, 6)	(16, 8)	(16, 6)	(12, 7)
	Sensitivity (s/m)	55.67	55.67	47.00	46.96	42.40

study, involves tournament selection and uniform crossover.

This study selects a set of GA parameters based on previous studies (McKinney and Lin 1994; Wang and Zheng 1998; Chang et al. 2007) for performance analysis of the algorithm with various parameters and attempts finding suitable parameters. In the study, the GA parameters are as follows. Maximum number of generations in the program is 100. Population size is 500 chromosomes. Rate of crossover is 0.8. Mutation probability is 0.01.

Numerical results and discussion

Observation network design problem

Numerical analyses on a hypothetical case were performed to verify the effectiveness of the proposed methodology. A hypothetical, homogeneous, isotropic confined aquifer serves as an

example. Figure 2 presents the finite difference meshes with dimensions of 13×19 . The mesh interval is equal to 500 m. The example associates with no-flow boundary conditions to the north and south of the aquifer, and constant-head boundaries to the west and east with hydraulic heads of 50 and 20 m. True value of transmissivity (T1) is assumed to be $3.0 \times 10^{-2} \text{ m}^2/\text{s}$. In problem 1, the decision variable is the new observation location. The location of existing observation wells are (5, 4), (5, 10), (15, 4), and (15, 10). The origin (0, 0) is at the above left in the domain. The number of candidate observation wells is 183. The model minimizes the estimated covariance while limiting fixed cost, with the number of newly designed observations limited to five. In addition, the minimum distance between two newly designed observations is 1,000 m. Various pumping well locations are selected in the aquifer. The location of the existing pumping well is at (5, 7) in case 1, (10, 7) in case 2, and at (15, 7) in case 3.

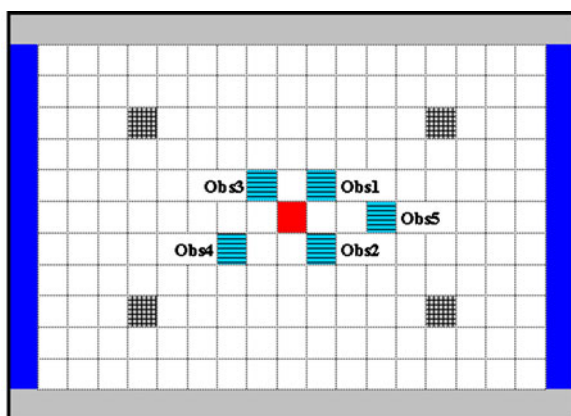


Fig. 3 Results in case 2

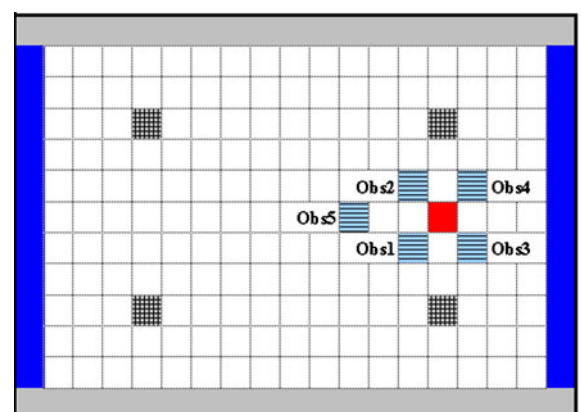


Fig. 4 Results in case 3

Table 2 Optimal location of pumping well and estimated transmissivity

	Optimal pumping well location	Pumping well at T1 or T2 zone	Estimated T1 (m ² /s)	Relative error	Estimated T2 (m ² /s)	Relative error
Case 4	(5, 9)	T1	1.98×10^{-2}	1.0%	3.82×10^{-2}	4.5%
Case 5	(4, 3) (6, 5)	T1	1.98×10^{-2}	1.0%	3.84×10^{-2}	4.0%

Table 1 presents the newly designed observations. The estimated parameter in the model is equal to the transmissivity (T1). In case 1, the locations of the newly designed observation wells are (4, 6), (4, 8), (6, 5), (6, 8) and (8, 7); in case 2, they are (8, 8), (9, 6), (11, 6), (11, 8), and (13, 7); in case 3, they are (12, 7), (14, 6), (14, 8), (16, 6), and (16, 8). Figures 2, 3, and 4 present the networks of observation network designs. Clearly, the newly designed observation network depends on pumping network locations. Table 1 also shows sensitivity in the newly designed observation (Obs1–Obs5). Results demonstrate that optimal observation location is most sensitive in all candidates. This finding reveals that the sensitivity decreases proportionally to the distance to the pumping well. Therefore, sensitivity increases with closer observation to the pumping well, reducing parameter evaluation uncertainty. The observation wells are firstly designed in the sensitive flow field to minimize uncertainty of estimated parameter values. The results confirm the previous study that the observation network for the transmissivity field is guided on the basis of the ar-

eas of the high hydraulic head gradient, since the information from the areas will lead to the most reliable management strategy (Andricevic 1990, 1993). The GA finds the optimal observation well effectively with various pumping well locations and is flexible in manipulating the highly complex spatial distribution. Moreover, when optimal observation network is determined, the information provided by the design is sufficient. The information is sufficient for parameter estimation so that the reliable parameters are identified (Chang et al. 2005).

Pumping network design problem

Following the above example, the decision variable in this design is only the pumping well location with 183 candidate sites. Existing observation wells are located at (5, 4), (5, 10), (15, 4), and (15, 10). Various numbers of pumping well designs demonstrate the cases. In the cases, case 4 designs a single pumping well, while case 5 designs two pumping wells. The pumping rate for each well is assumed to be 0.5 m³/s.

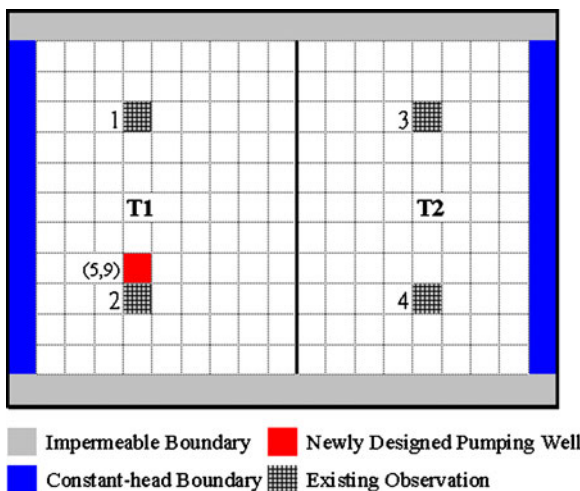


Fig. 5 Results in case 4

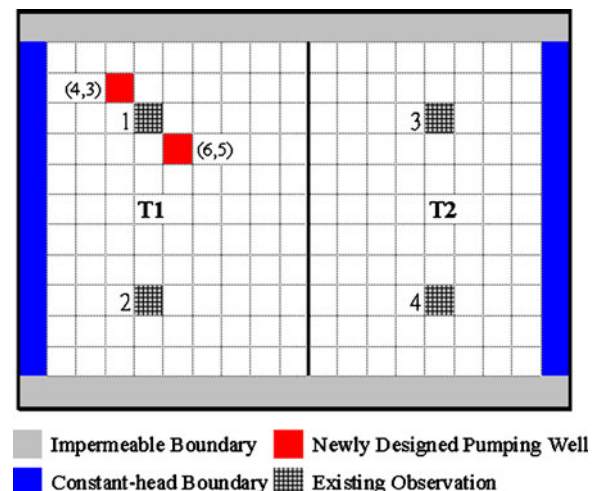


Fig. 6 Results in case 5

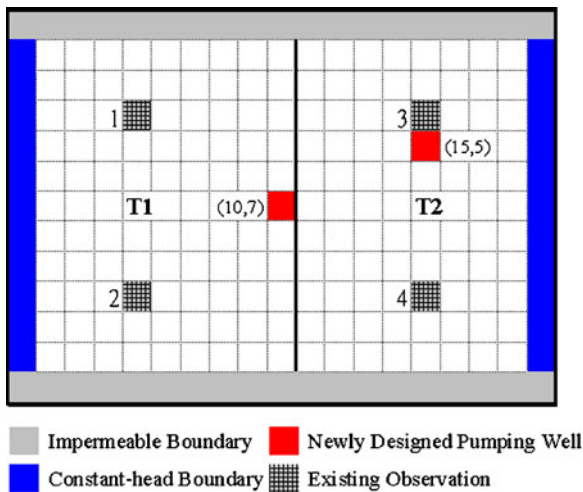


Fig. 7 Plan view in cases 6b and 6c

Table 2 lists case conditions and optimization results. The optimal pumping location obtains parameter values (T1, T2), as presented in Table 2 below. Transmissivity in case 4 is estimated as $T1 = 1.98 \times 10^{-2}$ and $T2 = 3.82 \times 10^{-2}$ m²/s by UCODE, with relative errors of 1% and 4.5%. Estimated transmissivity in case 5 is $T1 = 1.98 \times 10^{-2}$ and $T2 = 3.84 \times 10^{-2}$ m²/s and relative errors are 1% and 4%. Results demonstrate that the optimal pumping well location in case 4 is (5, 9), as presented in Fig. 5. Optimal pumping well locations in case 5 are at (4, 3) and (6, 5) in Fig. 6. Results also indicate that the optimal well locations in both cases are in the zone T1. Results reveal that the pumping network is sensitive to geological conditions. Pumping wells are designed in the sensitive geological zone to increase experimental design reliability. Thus, the network design provides the sufficient information for reliable estimation when the network is firstly located in the sensitive geological zone (Chang et al. 2005). Furthermore, the required average CPU time for

above cases is 16,308 s (4.5 h) on AMD CPU (K7—1 GHz).

This work compares parameters estimated by the optimal pumping network with those estimated by other pumping networks to verify that the optimal pumping network obtained in case 4 is an efficient network design for estimating practical-situation parameters. The pumping site of case 6a locates at (5, 9) following case 4 (Fig. 5). Pumping wells in cases 6b and 6c are randomly chosen at (10, 7) and (15, 5), as presented in Fig. 7. This work obtains the observed hydraulic head estimating the parameters in these cases by adding the simulated head to the head noise generated at the observation sites. The head noise is generated using standard normal distribution with zero mean and standard deviation of 0.1. The observation data are then used to estimate parameters using UCODE.

Table 3 presents the estimated parameters for the validation. In case 6a, the relative error when compared to true parameter values is 3.0% in optimal pumping network. In case 6b, the relative errors are 48.5% and 43.5%. In case 6c, the relative errors are 13.5% and 12.5%. A comparison of relative errors reveals that, among three cases, case 6a has the lowest estimation error. This result reveals that the design using GA is substantially better and transmissivity is accurately estimated based on effective information by applying the GA. Furthermore, by the two-level formulation, the discrete nature of the original problem is considered in the problem and facilitates the application of other computational efficient algorithms to solve the parameter estimation problem (sub-problem) and thus reduce the computational burden. This study uses the GA to solve the main problem and the GA accomplishes the discrete nature of searching for optimal well network alternatives. Within the GA, each chromosome

Table 3 Estimated T1 and T2 under various pumping locations

Case	Location of pumping well	Estimated T1 (m ² /s)	Relative error	Estimated T2 (m ² /s)	Relative error
Case 6a	(5, 9)*	2.06×10^{-2}	3.0%	4.12×10^{-2}	3.0%
Case 6b	(10, 7)	1.03×10^{-2}	48.5%	2.26×10^{-2}	43.5%
Case 6c	(15, 5)	1.73×10^{-2}	13.5%	3.52×10^{-2}	12.0%

*represents the optimal design case

(network design) associates a sub-problem which contains nonlinear characteristics. The GA is more effective in finding a nearly global optimal solution in the problem with integer variables when compared to conventional gradient-based optimization methods (Sciortino et al. 2002).

Conclusions

This study explores mathematical characteristics of the regional groundwater network design and reformulates it as a two-level optimization problem to facilitate the GA and modified Gauss–Newton algorithm application. Based on the formulation, discrete decision variables of the problem are solved in the main-problem using the GA, while continuous decision variables of the problem are computed in the parameter estimation problem using the modified Gauss–Newton algorithm. The methodology is developed to minimize uncertainty of the estimated aquifer parameters (transmissivity) by selecting optimal locations of the observation or pumping network. The GA determines the number and locations of observation and pumping wells; then, the parameters are estimated for a given network design using Gauss–Newton algorithm.

Results indicate that GA successfully solves the experimental design problem, confirmed in numerical experiments in which the proposed method is computationally efficient. This study adopts this fundamental approach to demonstrate that the design yields a reliable transmissivity value. This approach further investigates two points. First, observation wells are designed close to the sensitive flow field to minimize uncertainty of estimated parameter values. Second, locating pumping wells in the least transmissivity zone ensures much sensitivity, and effectively designs pumping wells in the least transmissivity zone. Other suggestions follow.

The traditional experimental design is a sequential design. The optimal design is found only for each stage, not for all stages. The multi-stage design is favorable for long-term groundwater planning. The design policies in total stages should be regarded as experimental design guidelines.

A complete regional field investigation of aquifer parameters should include two main stages, regional network planning and on-site pumping test design. The most rational approach integrates the sampling design procedure into an experimental design. Future studies could further study observation frequency and duration. This work recommends that future studies clarify the relationship between total cost and transmissivity uncertainty to determine a trade-off between the two.

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