Determination of the parameter pattern and values for a one-dimensional multi-zone unconfined aquifer

Ya-Chi Chang · Hund-Der Yeh · Yen-Chen Huang

Abstract In an aquifer, heterogeneity plays an important role in governing groundwater flow. Hence, aquifer characterization should involve both the pattern and values of the hydrogeological parameters. A new analytical solution describing the one-dimensional groundwater flow in a multi-zone unconfined aquifer is presented, and a methodology developed from the analytical solution and a heuristic approach for determining the pattern and values of the aquifer parameters are proposed. The analytical solution demonstrates that the hydraulic head varies spatially and is influenced by aquifer heterogeneity. Simulated annealing, a heuristic approach, is incorporated with the solution to simultaneously identify the pattern and values of the hydraulic conductivity for a horizontal multi-zone unconfined aquifer. This approach may be used to give an approximate result for a two-dimensional problem by dividing the model area into a number of transects along the transverse direction, identifying the parameter values along the longitudinal direction for each transect, and then smoothing the identified results.

Résumé Dans un aquifère, l'hétérogénéité joue un rôle important en gouvernant l'écoulement des eaux souterraines. En conséquence, la caractérisation de l'aquifère devrait inclure et l'espace et les valeurs des paramètres hydrogéologiques. Une nouvelle solution analytique décrivant l'écoulement des eaux souterraines uni-dimensionnel dans un aquifère non-confiné à plusieurs couches est présenté, et la méthodologie développée à partir de la solution analytique et une approche heuristique pour déterminer l'espace et les valeurs des paramètres de l'aquifère sont proposées. La solution analytique démontre que la charge hydraulique varie spatialement et est influencée par l'hétérogénéité de l'aquifère. Le « recuit simulé », une approche heuristique d'optimisation, est incorporé avec la solution pour identifier simultanément l'espace et les valeurs de conductivités hydrauliques pour un aquifère libre horizontal et multi-zones. Cette approche peut être utilisée pour donner un résultat approximatif pour un problème bidimensionnel en divisant l'aire du modèle en une suite de plusieurs sections, identifiant les valeurs de paramètre le long de la direction longitudinale pour chaque section, et ensuite en arrondissant les résultats.

Resumen En un acuífero, la heterogeneidad juega un papel importante en el flujo del agua subterránea. Así, la caracterización de un acuífero debe tener en cuenta tanto la disposición como los valores de los parámetros hidráulicos. Se presenta un nueva solución analítica que describe el flujo del agua subterránea en una dimensión en un acuífero libre multi-zona, y se propone una metodología desarrollada a partir de la solución analítica y la aproximación heurística para determinar la disposición y los valores de los parámetros del acuífero. La solución analítica demuestra que el nivel piezométrico varía espacialmente y está influenciado por la heterogeneidad del acuífero. Un templado simulado, una aproximación heurística, se ha incorporado a la solución para identificar simultáneamente la disposición y los valores de la conductividad hidráulica para un acuífero libre horizontal multi-zona. Esta aproximación puede ser utilizada para proporcionar un resultado aproximado en un problema bidimensional dividiendo el área del modelo en un número de transectos a lo largo de la dirección transversa, identificando los valores del parámetro a lo largo de la dirección longitudinal para cada transecto, y entonces suavizando los resultados identificados.

Keywords Groundwater flow · Hydrogeological parameter · Analytical solutions · Multi-zone unconfined aquifer · Simulated annealing

Received: 13 June 2006 / Accepted: 20 September 2007
Published online: 19 October 2007

Y.-C. Chang · H.-D. Yeh (✉) · Y.-C. Huang
Institute of Environmental Engineering,
National Chiao Tung University,
No. 75, Po-Ai Street, Hsinchu, 300, Taiwan
e-mail: hdyeh@mail.nctu.edu.tw
Tel.: +886-3-5731910
Fax: +886-3-5726050
Y.-C. Chang

e-mail: rachel.ev91g@nctu.edu.tw
Y.-C. Huang

e-mail: boyz.ev89g@nctu.edu.tw

 DOI 10.1007/s10040-007-0228-3

Introduction

It is important to understand the aquifer characteristics when dealing with groundwater problems, since aquifer parameters such as hydraulic conductivity and storage coefficient are the key properties in characterizing the aquifer formation. In groundwater modeling, hydraulic conductivity is the most important hydrogeological parameter for describing the ease with which water flows through a porous medium. The hydraulic parameters can be quantified through calibration by simulating the hydraulic heads at an observation well. Although hydraulic head is often described in pumping test analysis by equations such as the Theis equation for confined aquifers and the Boussinesq equation for unconfined aquifers (Schwartz and Zhang 2003), both equations require the assumption of a homogeneous aquifer, i.e., the hydraulic conductivity is the same everywhere in the aquifer. However, in a horizontal multi-zone unconfined aquifer, the number of zones and the hydraulic conductivity of each zone will affect the groundwater flow. In addition, the heterogeneous hydraulic conductivity may complicate the groundwater flow estimation and result in incomplete spatial distribution of the hydraulic head. In order to better understand the groundwater flow in a heterogeneous aquifer, parameter identification is often inevitable in hydrogeological sciences. The concept of the inverse problem for groundwater modeling and parameter identification were intensively reviewed by Marsily et al. (1999) and Carrera et al. (2005).

Parameter structure identification may involve both the pattern and values of the aquifer parameters. However, previously the parameter pattern was usually defined prior to parameter value estimation (Yeh 1986). In general, the parameter pattern was estimated in a trial-and-error manner since prior information on the aquifer was always limited. Although the trial-and-error approach is flexible, it is time-consuming and the solution is strongly dependent on the skill of the practitioner (Keidser and Rosbjerg 1991). Zheng and Wang (1996) carried out a fairly intensive review of parameter structure identification. They realized that the development of an efficient and systematic procedure for parameter pattern estimation remains a challenging area of research, and the combined optimization of both parameter pattern and parameter values is even more difficult.

In the past, methods using the least-square approach were commonly employed to estimate aquifer parameters (e.g., Yeh 1987; Yeh and Han 1989). However, two problems arise when employing gradient-type methods to solve the least-square equations. First, these methods may yield diverging results if the guessed parameter values are not very close to the target values. Second, these methods may yield poor results if incorrect increments have been used when applying the finite difference formula to approximate the derivative terms. To resolve this, global optimization methods using heuristic search techniques have emerged rapidly in recent years. Simulated annealing (SA) is one of the major optimization methods. The theory of SA was developed by Metropolis et al. (1953), who introduced a simple algorithm to incorporate the idea of the behavior of a particle system in thermal equilibrium into numerical calculations of an equation state. SA is a random search algorithm that allows, at least in theory or in probability, the global optimum of a function in any given domain to be obtained. This theory was first applied to a number of problems arising in optimal design of computers by Kirkpatrick et al. (1983) and to the area of groundwater management by Dougherty and Marryott (1991).

Existing studies on parameter structure identification combined optimization methods with numerical approaches such as finite difference or finite element methods to identify hydrogeological parameters. However, it is cumbersome and laborious to re-discretize the domain for numerical methods when SA generates each new trial solution for the parameter pattern. For this reason, parameterization (e.g. zonation and interpolation) must be employed to approximate the spatial distribution of aquifer parameters when incorporating the numerical models with SA to identify the parameter structure. Zheng and Wang (1996) used the finite difference method to approximate the transient groundwater flow equation and used the zonation method to identify the parameter structure. They focused on the identification of parameter structure by treating the number of zones and the hydraulic conductivity for each zone as known, and divided the problem domain into several nodal points with a regular spacing. However, their approach is not applicable to the case where the unknown boundaries of the parameter zones are not located at the nodal points. In reality, the zone boundaries are usually unknown and not distributed regularly. The numerical methods might obtain results with poor accuracy if improper grids were used when applying the parameterization methods. It may practically be impossible to assign the nodal points right at the zone boundaries since they are unknown. In addition, the numerical methods introduce numerical errors such as truncation and round-off errors.

A new analytical solution for describing the groundwater flow for a one-dimensional multi-zone unconfined aquifer is derived in this paper. The analytical solution allows discontinuity for the head and hydraulic conductivity at the zone boundary. However, the gradient-type approaches such as Newton's method and the Gauss-Marquart method, require the objective function to be continuous at the zone boundary. Thus, SA is proposed together with the derived analytical solution to determine the optimal parameter pattern and values simultaneously in a one-dimensional multi-zone unconfined aquifer. This approach may also be used to give an approximate result for a two-dimensional problem by dividing the model area into a number of transects along the transverse direction, identifying the parameter values along the longitudinal direction for each transect, and then smoothing the identified results. The analytical solution is derived from

 DOI 10.1007/s10040-007-0228-3

Darcy's law and the groundwater flow equation and then coupled with the SA to identify simultaneously the parameter pattern and values. This solution can describe the spatial distribution of the hydraulic head in a heterogeneous unconfined aquifer with recharge. The proposed approach is convenient and flexible for identifying the parameter pattern and values by combining the SA with the new analytical solution. Several different cases for simulating real-world problems are considered and the results indicate that the parameter pattern and values for a one-dimensional horizontal multi-zone unconfined aquifer are simultaneously and accurately identified by the proposed approach.

Methodology

Analytical solution

An aquifer is considered to be homogeneous if the permeability in a given direction is the same from point to point in a geological unit. Alternatively, materials that do not conform to this condition are heterogeneous (Schwartz and Zhang 2003). A simple example of heterogeneity in permeability is represented by a zoned geological unit with variable hydraulic conductivities.

As shown in Fig. 1, the hydraulic head and the flow rate per unit width in the ith zone of the horizontal multi-zone unconfined aquifer with recharge are

$$h_i(x) = \sqrt{-wx^2 \Big/ K_i + \lambda x \Big/ K_i + \sum_{j=1}^{i} \Delta k_j \lambda x_{j-1} + w \sum_{j=1}^{i} \Delta k_j x_{j-1}^2 + h_0^2} \tag{1}$$

and

$$q_i^{'}(x) = wx - \lambda/2 \tag{2}$$

where

$$\lambda = \frac{\left[\sum_{i=1}^{n} w\left(x_i^2 - x_{i=1}^2\right) \Big/ K_i\right] + \left(h_L^2 - h_0^2\right)}{\sum_{i=1}^{n} \left(x_i - x_{i-1}\right) \Big/ K_i} \tag{3}$$

and

$$\Delta k_j = \left(1/K_j - 1/K_{j+1}\right) \tag{4}$$

The detailed derivations of Eqs. (1) and (2) are presented in the Appendix.

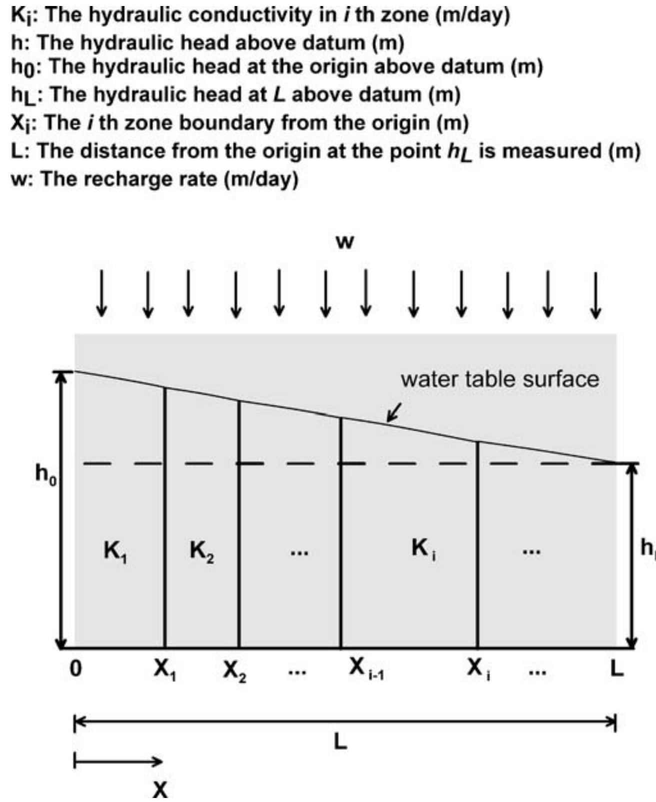


Fig. 1 A cross-section of groundwater flow in a horizontal multi-zone unconfined aquifer with recharge

Simulated annealing

Metropolis et al. (1953), the forerunner in SA, applied the methodology in a two-dimensional rigid-sphere system. Kirkpatrick et al. (1983) had the innovative idea of using SA to solve large-scale combined optimization problems. Since then, SA has been applied in many engineering optimization problems (Dougherty and Marryott 1991; Romeo and Sangiovanni-Vincentelli 1991, Marryott et al. 1993, Aarts et al. 1997, Cunha and Sousa 1999). The basic algorithm of the annealing process is to heat up an object from solid phase to liquid phase and then let it cool down slowly. As the temperature is reduced, the atomic energies decrease. While it is crystallized, the system energy of the object will be in the minimum state. Based on the annealing concept, SA was developed for solving optimization problems. The Metropolis's criterion (Kirkpatrick et al. 1983) is used in SA procedure to avoid the solution to be trapped in a local optimal solution.

The framework of SA is illustrated in Fig. 2. The first step is to initialize the initial solution and set the initial solution as being the current optimal solution. The second step is to update the current optimal solution, if the trial solution generated from the initial solution within the boundary is better than the current optimal solution or if the trial solution satisfies the Metropolis's criterion; otherwise, continue generating the trial solution. Usually, after a specified number of algorithm iterations, n_1, are performed, the temperature will be decreased by the temperature reduction factor R_t, even if no improvement

DOI 10.1007/s10040-007-0228-3

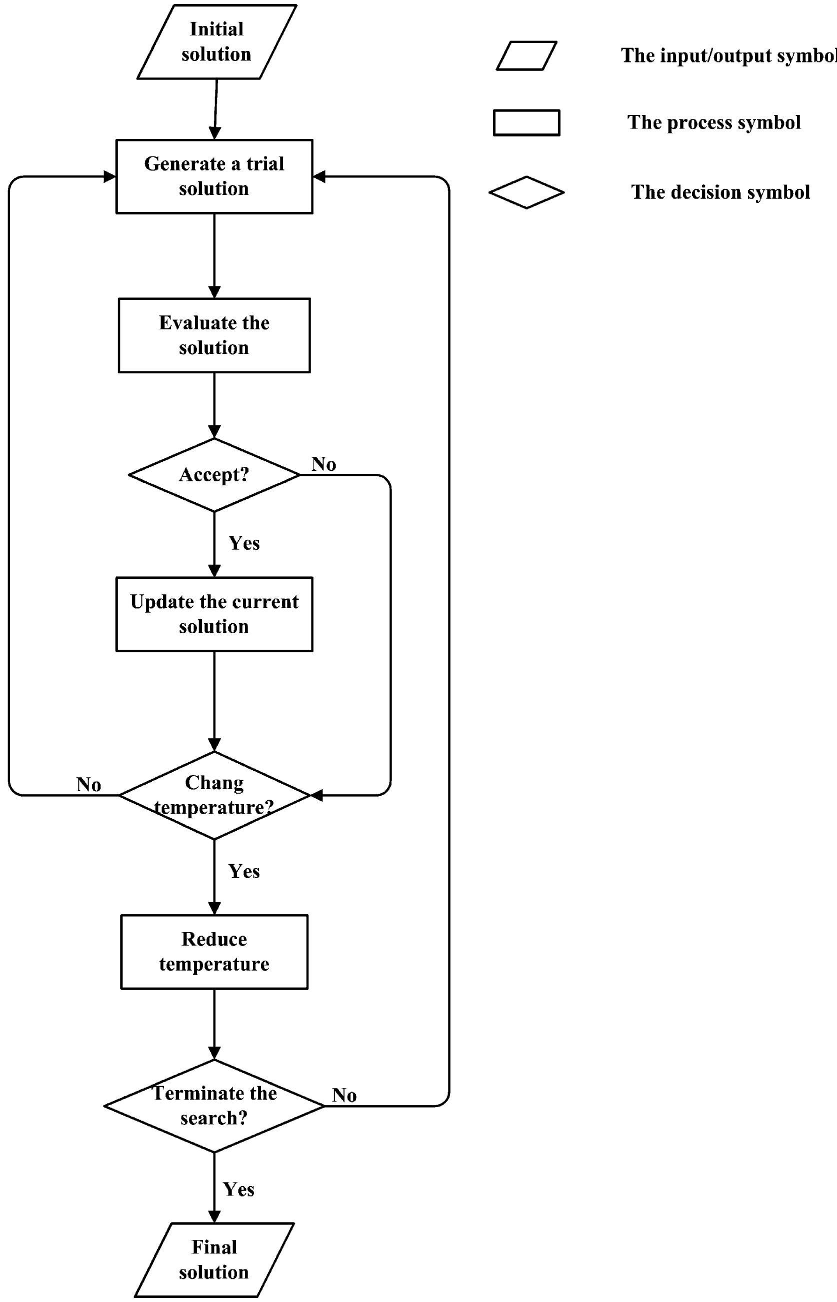


Fig. 2 Flowchart of simulated annealing (SA) (modified from Yeh et al. 2007)

of the optimum takes place. The temperature should be allowed to cool properly to guarantee the obtained solution is the global optimal solution. The algorithm will be terminated when SA obtains the optimal solution or the obtained solution satisfies the stopping criteria. In general, the stopping criteria are defined to check whether the temperature or the difference between the optimal objective function value and those obtained in the current iteration reaches the specified value or not.

The values of hydraulic conductivity K_i and zone boundary x_i between zone (i) and zone (i+1) for a multi-zone unconfined aquifer are identified when employing SA to analyze the simulated hydraulic head data. Several cases are discussed in this paper. The aquifer parameters may be estimated from the solution of a multi-zone unconfined aquifer while minimizing the sum of square errors between the observed and predicted heads. Therefore, the objective function is defined as

$$Minimize \sum_{i=1}^{m} (Oh_i - Ph_i)^2 \tag{5}$$

where Oh_i and Ph_i are, respectively, the observed and predicted heads at different positions, and m is the number of observed data.

Figure 3 illustrates a brief schematic explaining how to apply SA coupled with the derived analytical solution to

DOI 10.1007/s10040-007-0228-3

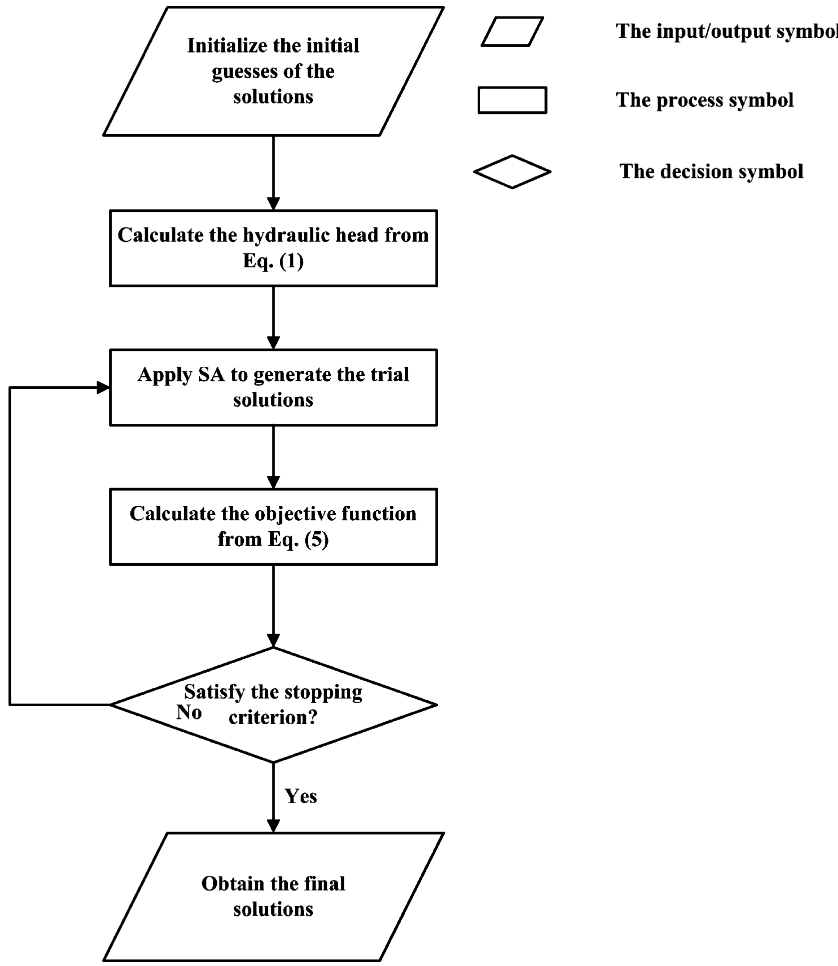


Fig. 3 The parameter identification procedure (modified from Yeh et al. 2007)

identify aquifer parameters. The related procedure is as follows:

Step 1. Initialize the initial guesses of the aquifer parameters.
Step 2. Calculate the predicted head based on Eq. (1).
Step 3. Apply SA to generate the trial solutions (aquifer parameters). Note that the algorithmic parameters in SA need to be specified in this step. The current optimal solution at each annealing state will be obtained from all possible solutions (trial solutions) based on Metropolis's criterion.
Step 4. Check the obtained results. After the objective function value meets the specified stopping criterion, SA is terminated as the optimal solution is obtained. Otherwise, return to step 3 to keep on generating possible solutions.

Notice that the FORTRAN (mathematical formula translation system) code of SA used in this study was originally developed by Goffe (1995).

Results and discussion

To test the applicability of the proposed approach, several cases for simulating a real-world problem over a 1,000 m length are considered. The hydraulic head on the right-hand side (RHS) and left-hand side (LHS) are, respectively, 10 and 11 m; and the average recharge rate is 0.00034 m/day in these cases. In addition, Table 1 lists the target values of hydraulic conductivities and zone boundaries for sets A, B and C. The details of the control elements in SA are described below. In order to avoid having negative conductivity, the lower and upper bounds of hydraulic conductivity for each zone are set to be 10^{-4} and 5,000 m/day, respectively. The initial temperature of the SA method is 100 in this study. The temperature is dimensionless and is decreased by the temperature reduction factor (0.85) after 8,100 calculations. The annealing process will be terminated if the absolute differences between two successive objective function values are all less than 10^{-10} within 20 iterations or the number of evaluations is greater than 10^{7}.

Constraints for number and location of observation wells

For an n-zone aquifer, there should be at least $2n$-1 observations to determine $2n$-1 unknowns of n hydraulic conductivities and n-1 locations of the zone boundaries. In addition, at least one observation well is required in each

 DOI 10.1007/s10040-007-0228-3

Table 1 The target hydraulic conductivities and zone boundaries for sets A, B and C

Set	Hydraulic conductivity (m/day)				Zone boundary from origin (m)		
	K_1	K_2	K_3	K_4	x_1	x_2	x_3
A	2513.2	543.8	50.86	1023.5	250.8	601.9	814.6
B	17.25	3084.5	201.53	50.9	124.32	204.6	912.1
C	17.25	3084.5	201.53	50.9	124.32	204.6	912.1

zone to uniquely determine the unknown hydraulic conductivity in that zone.

A four-zone aquifer with different locations of observation well

Two cases, cases A1 and A2, are chosen to investigate the influence of locations of the observation wells on the analyzed results of the proposed approach. The four-zone aquifer has a length of 1,000 m and the zone boundaries are located at 250.8, 601.9 and 814.6 m from the origin, respectively. The symbol "A1" indicates the case is assumed with the target hydraulic conductivities and zone boundaries for set A as listed in Table 1 and with observation network 1 as listed in Table 2. Table 1 shows the target hydraulic conductivities for zones 1 to 4 as 2,513.2, 543.8, 50.8 and 1,023.5 m/day and Table 2 lists the observation networks for these two cases. Seven observation wells are placed at 125, 250, 375, 500, 625, 750 and 875 m from origin in case A1. All observation wells in case A1 have an equal spacing of 125 m. The observation wells are placed arbitrarily at 160.34, 201.91, 291.54, 513.92, 752.34, 813.51 and 945.35 m in case A2.

The identification results obtained from the present approach are listed in Table 3. The estimated locations for the zone boundaries are deduced extremely well in these two cases. In case A1, the estimated hydraulic conductivities have relative errors of about 1%. In case A2, which has better results, the relative errors of estimated conductivities are all less than 0.1%. Although the locations of observation wells are different between cases A1 and A2, the estimated locations of the zone boundaries are excellent and the estimated hydraulic conductivities are reasonably good when compared with the target values listed in Table 1. It is noted that the objective function values of these two cases are very small as indicated in Table 3. In addition, Fig. 4 illustrates that the predicted heads conform to the observed heads and the proposed approach works very well in these two cases.

A four-zone aquifer with observed hydraulic heads with noise

Case A2a is performed to test the capability of the proposed approach when determining simultaneously the structure and value of the aquifer parameters for real-world problems. The characteristics of the aquifer and the location of observation wells in case A2a are similar to those in case A2, but the observed hydraulic head data contains white noise, which is generated by MATLAB (The MathWorks 1995). The MATLAB function randn(m, n) is an m-by-n matrix, chosen from a normal distribution with mean zero, variance one and standard deviation one (The MathWorks 1995). In this study, $m=1{,}000$ and $n=1$ is chosen to generate a realization of white noise (Leng and Yeh 2003). The elements in this realization are normally distributed as random numbers with zero mean and unit variance. Seven elements are taken from this realization and each element is then multiplied by 1.0×10^{-3}, with the assumption that the measurement errors are in the order in millimeter. The results for the estimated hydraulic conductivity and zone boundaries for case A2a are also listed in Table 3. The estimated hydraulic conductivities are 2,499.9, 573.1, 53.3 and 1,068.2 m/day, and the estimated zone boundaries are 252.4, 602.0 and 814.6 m in case A2a. The objective function value is 3.71×10^{-7} in case A2a. The results for case A2a are fairly close to the target values indicating that SA may also be applicable for field data, although the objective function is slightly higher than those in the previous cases.

A four-zone aquifer with different properties

Case B is for a four-zone aquifer with the target hydraulic conductivities and zone boundaries given in Table 1 as set B. The hydraulic conductivities are 17.25, 3,084.5, 201.53 and 50.9 m/day for those four zones and the locations are 124.32, 204.6, and 912.1 m, respectively, for the zone boundaries 1–3. The observation wells are arranged as those in case A2. The results for case B are also listed in

Table 2 The location for observation networks 1 and 2

Network	Location of observation well measured from origin (m)						
	OW_1	OW_2	OW_3	OW_4	OW_5	OW_6	OW_7
1	125.00	250.00	375.00	500.00	625.00	750.00	875.00
2	160.34	201.91	291.54	513.92	752.34	813.51	945.35

Note that OW_i is the ith observation well.

Table 3 Results for cases A1, A2, A2a, B and C using simulated annealing (SA)

Case	Hydraulic conductivity (m/day)				Zone boundary from origin (m)			Objective function	Computing time (hr)
	K_1	K_2	K_3	K_4	x_1	x_2	x_3		
A1	2545.6 (1.2%)[a]	550.4 (1.2%)	51.4 (1.1%)	1035.0 (1.1%)	250.8 (0%)	601.9 (0%)	814.6 (0%)	9.04×10^{-13}	0.95
A2	2516.0 (0.1%)	544.3 (0.09%)	50.9 (0.07%)	1024.4 (0.08%)	250.7 (0.04%)	601.9 (0%)	814.6 (0%)	4.85×10^{-14}	0.94
A2a	2499.9 (0.5%)	573.1 (5%)	53.3 (4.7%)	1068.2 (4.3%)	252.4 (0.63%)	602.0 (0.01%)	814.6 (0%)	3.71×10^{-7}	0.98
B	16.8 (2.6%)	3083.3 (0.03%)	201.5 (0.01%)	50.8 (0.19%)	121.1 (0.02%)	204.6 (0%)	912.1 (0%)	4.21×10^{-14}	0.95
C	17.2 (0.28%)	3083.9 (0.01%)	201.5 (0.01%)	50.9 (0%)	124.3 (0.01%)	204.6 (0%)	912.1 (0%)	9.86×10^{-13}	12.5

[a] The relative error of the estimated parameter value

Table 3. The estimated hydraulic conductivities are 16.8, 3083.3, 201.5 and 50.8 m/day, and the estimated zone boundaries are 121.1, 204.6 and 912.1 m in case B. The relative errors of estimated conductivities and zone boundaries are all less than 2.6% and the objective function value is 4.21×10^{-14} in case B. The results obtained from case B indicate that the proposed approach gives good estimations when identifying the parameter values and pattern for various aquifers.

Identification of number of zones

The target values of hydraulic conductivity and the locations of the zone boundaries for case C are the same as those in case B. However, the number of zones in case C is unknown at the beginning and the proposed approach is utilized to determine the number of zones, the parameter pattern and values at the same time. To avoid violating the constraints for the number and location of observation wells, a maximum number of eight zones are considered in case C. Thus, 15 observation wells are chosen to be uniformly distributed with an interval of 62.5 m along the length of the aquifer. The proposed approach is employed to analyze such an observed data set when considering the number of zones, which ranges from 1 to 8. Figure 5 illustrates the estimated objective function value versus different numbers of zones in case C. This result clearly indicates that the proposed approach properly identifies the number of zones in the aquifer; in other words, the optimal result coincides with the real pattern of the aquifer. Table 3 displays the optimal results of estimated parameters in case C. The estimated hydraulic conductivities are 17.2, 3,083.9, 201.5 and 50.9 m/day, and the estimated zone boundaries are 124.3, 204.6 and 912.1 m. The objective function value is 9.86×10^{-13} for the optimal result, which is close to the target value in case C.

A fifty-zone aquifer

Case D is designed to assess the performance of the proposed approach when applied to an aquifer with trending heterogeneity. The hydraulic head on the RHS and LHS and the average recharge rate are the same as previous cases. The aquifer hydraulic conductivities are expressed as and (m/day) for the target values where *i, j* denote the *i*th and *j*th zone and $i=1,2,3...,25$; $j=26,27,28...50$. It is assumed that each zone has an equal spacing of 20 m. The results indicate that the relative errors of the estimated zone boundaries are less than 0.3% and the relative errors of estimated conductivities are less than 1.9% except the 28th layer. The estimated conductivity of the 28th layer is 1,134.6 m/day with the target value of 940 m/day. The objective function value is 2.18×10^{-9} for the optimal result, which is also close to the target value in case D. The objective function value is higher than those in the other cases since the observation values are also more.

All the estimated hydraulic conductivities and zone boundaries are fairly close to the target values in the five cases shown in Table 3. The results in cases A1 and A2 demonstrate that the proposed approach identifies accurately the parameter pattern and values with different locations of observation wells. The results in case B show that the proposed approach is suitable for the varying characteristics of aquifers. The value of the objective function in case A2a is higher than that in other cases due to the noise in the observations. Obviously, the proposed approach can be employed to identify simultaneously the parameter pattern and values when the number of zones is unknown as shown in case C. In case D, although the number of unknown parameters is much greater than in the other cases, the parameters can be identified accurately by the proposed approach.

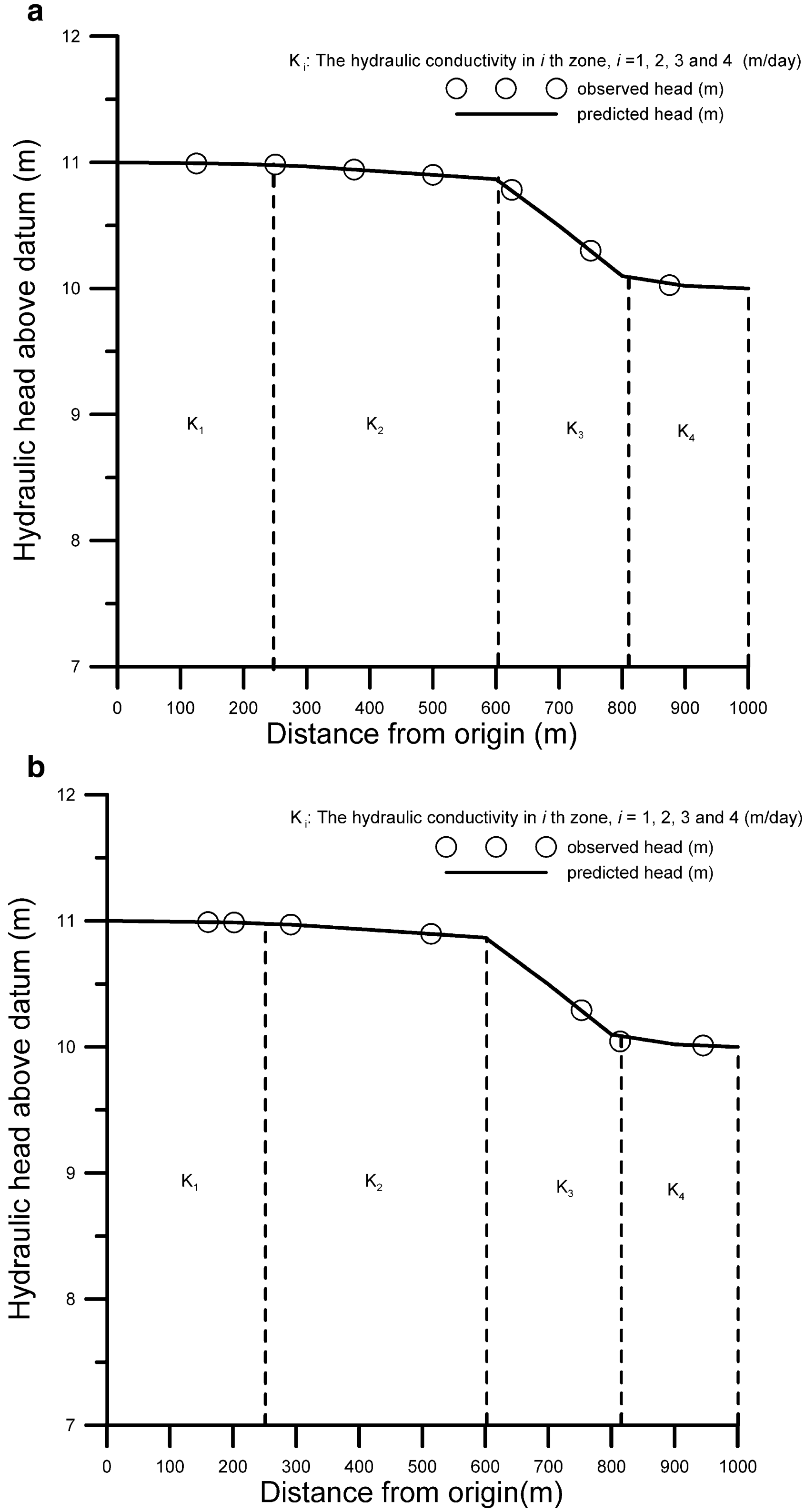
The computing times for different cases are also listed in Table 3. The parameter estimation took about one hour and 7×10^{7} iterations for cases A1, A2, A2a and B on a Pentium IV 3.2 GHz machine. For case D, it took less than 18 h and about 9×10^{8} iterations. Case D took more time and required more iterations because the identified parameters were many more than those of other cases.

Summary and conclusions

A new analytical solution is derived to describe the hydraulic head distribution in a one-dimensional heterogeneous unconfined aquifer with recharge at the top of the aquifer. This solution demonstrates spatial variation of hydraulic heads, which is strongly influenced by the

 DOI 10.1007/s10040-007-0228-3

Fig. 4 The observed heads and predicted heads in **a** case A1, **b** case A2



heterogeneous hydraulic conductivity and the zone boundary of each zone in the aquifer. Obviously, parameter identification for groundwater modeling should include both the pattern and values of the parameters for a heterogeneous aquifer.

In order to identify the parameters for groundwater, a new approach, incorporating SA with the analytical solution, is proposed to identify the parameter pattern and values simultaneously for a horizontal one-dimensional multi-zone unconfined aquifer including recharge. Five

 DOI 10.1007/s10040-007-0228-3

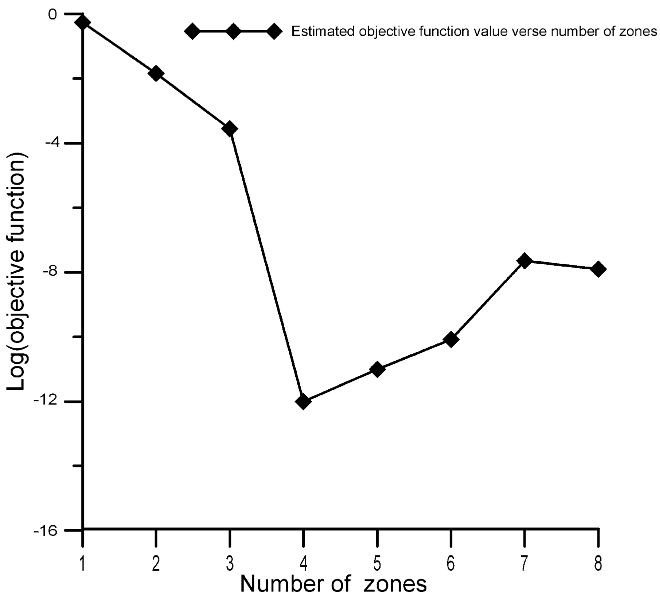


Fig. 5 The estimated objective function value versus number of zones for case C

cases are chosen to examine the applicability of the proposed approach. The estimated results demonstrate that the parameter pattern and values for horizontal one-dimensional multi-zone unconfined aquifers are appropriately identified without any prior information on the aquifer such as number of zones, hydraulic conductivity in each zone, and locations of zone boundaries. For site characterization, the proposed approach helps to determine simultaneously the pattern and values of hydrogeological parameters in horizontal multi-zone unconfined aquifers. The analytical solution is based on the assumption that each zone of the domain is homogeneous. For a large heterogeneous region, it serves as a useful tool for simultaneous identification of the parameter pattern and values in a one-dimensional multi-zone unconfined aquifer. In addition, the proposed approach may be used to give an approximate result for a two-dimensional problem by dividing the model area into a number of transects along the transverse direction, identifying the parameter values along the longitudinal direction for each transect, and then smoothing the identified results. However, such an approximation may not give good results if the aquifer is rather heterogeneous and the spacing of the transect is not very fine.

Acknowledgements This study was partly supported by the Taiwan National Science Council under grant NSC94-2211-E-009-015. The authors would like to thank the associated editor and two anonymous reviewers for their valuable and constructive comments.

Appendix

The equation for one-dimensional steady-state groundwater flow in a heterogeneous unconfined aquifer with recharge is

$$\frac{\partial}{\partial x}\left(K_i h_i \frac{\partial h_i}{\partial x}\right) + w = 0, i = 1, 2, ..., n \tag{6}$$

where h_i is the hydraulic head at x in the ith zone, x is the distance from the origin, K_i is the hydraulic conductivity in the ith zone, n is the number of zones and w is the recharge rate. Integrating Eq. (1) yields the expression

$$h_i^2 = -\frac{w}{K_i}x^2 + C_1 x + C_2 \tag{7}$$

where C_1 and C_2 are constants of integration. The left-hand side and right-hand side boundary conditions of the problem domain are, respectively,

$$h|_{x=0} = h_0 \tag{8}$$

and

$$h|_{x=L} = h_L \tag{9}$$

where h_0 is the hydraulic head at the origin, h_L is the hydraulic head at L, and L is the distance from the origin at the point h_L is measured. In addition, the continuity requirements for the hydraulic head and the flow rate per unit width at x_i are, respectively,

$$h_i(x_i) = h_{i+1}(x_i) \tag{10}$$

and

$$q_i'(x_i) = q_{i+1}'(x_i) \tag{11}$$

where $h_i(x_i)$ is the hydraulic head, x_i is the ith zone boundary, and $q_i'(x_i)$ is the flow rate per unit width at x_i in the ith zone. By solving the above equations, the hydraulic head and the flow rate per unit width in the ith zone of the horizontal multi-zone unconfined aquifer with recharge are therefore, respectively,

$$h_i(x) = \sqrt{-wx^2 \Big/ K_i + \lambda x \Big/ K_i + \sum_{j=1}^{i} \Delta k_j \lambda x_{j-1} + w \sum_{j=1}^{i} \Delta k_j x_{j-1}^2 + h_0^2} \tag{12}$$

and

$$q_i'(x) = wx - \lambda/2 \tag{13}$$

 DOI 10.1007/s10040-007-0228-3

where

$$\lambda = \frac{\left[\sum_{i=1}^{n} w\left(x_i^2 - x_{i-1}^2\right)/K_i\right] + \left(h_L^2 - h_0^2\right)}{\sum_{i=1}^{n} \left(x_i - x_{i-1}\right)/K_i} \tag{14}$$

and

$$\Delta k_j = \left(1/K_j - 1/K_{j+1}\right) \tag{15}$$

Equation (12) shows that the hydraulic head varies spatially and is influenced by the heterogeneous hydraulic conductivity of the multi-zone unconfined aquifer. When the aquifer is homogeneous, Eqs. (12) and (13) can, respectively, be reduced to (Fetter 1994)

$$h = \sqrt{h_0^2 - \frac{\left(h_0^2 - h_L^2\right)}{L} x + \frac{w}{K}(L - x)x} \tag{16}$$

and

$$q' = -Kh\frac{\partial h}{\partial x} = \frac{K\left(h_0^2 - h_L^2\right)}{2L} - w\left(\frac{L}{2} - x\right) \tag{17}$$

Note that Eq. (16) can be employed to find the elevation of the water table everywhere between two points located L distance apart if the saturated thickness of the aquifer is known at the two end points.

References

Aarts E, Korts J, Van Laarhoven PJM (1997) Simulated annealing. In: Aarts E, Lenstra JK (ed) Local search in combinatorial optimization. Wiley, Chichester, pp 91–120

Carrera J, Alcolea A, Medina A, Hidalgo J, Slooten LJ (2005) Inverse problem in hydrogeology. Hydrogeol J 13:206–222

Cunha MDC, Sousa J (1999) Water distribution network design optimization: simulated annealing approach. J Water Resour Plan Manage 125:215–220

Dougherty D, Marryott R (1991) Optimal groundwater management: 1. simulated annealing. Water Resour Res 27:2493–2508

Fetter CW (1994) Applied hydrogeology. Prentice-Hall, Englewood Cliffs, New Jersey, 691 pp

Goffe B (1995) Economics department, University of California, Berkeley. Software Archive. http://emlab.berkeley.edu/Software/abstracts/goffe895.html. Cited 8 Mar 2007

Keidser A, Rosbjerg DA (1991) A comparison of four inverse approaches to groundwater flow and transport parameter identification. Water Resour Res 24:670–682

Kirkpatrick S, Gelatt C, Vecchi M (1983) Optimization by simulated annealing. Science 220:671–680

Leng CH, Yeh HD (2003) Aquifer parameter identification using the extended Kalman filter. Water Resour Res 39:1062. DOI 10.1029/2001WR000840

Marryott AD, Dougherty DE, Stoller RL (1993) Optimal groundwater management, 2: application of simulated annealing to a field-scale contamination. Water Resour Res 29:847–860

Marsily G, Delhomme JP, Delay F, Buoro A (1999) 40 years of inverse problems in hydrogeology. Comptes Rendus Accad Sci, Sci Terre Planets 329:73–87

Metropolis N, Rosenbluth AW, Rosenbluth MN, Teller AH, Teller E (1953) Equation of state calculations by fast computing machines. J Chem Phys 21:1087–1092

Romeo F, Sangiovanni-Vincentelli A (1991) A theoretical framework for simulated annealing. Algorithmica 6:302–345

Schwartz FW, Zhang H (2003) Fundamentals of ground water. Wiley, New York, 583 pp

Yeh WWG (1986) Review of parameter identification procedures in groundwater hydrology: the inverse problem. Water Resour Res 22:95–108

Yeh HD (1987) Theis' solution by nonlinear least-squares and finite-difference Newton's method. Ground Water 25:710–715

Yeh HD, Han HY (1989) Numerical identification of parameters in leaky aquifers. Ground Water 27:655–663

Yeh HD, Lin YC, Huang YC (2007) Parameter identification for leaky aquifers using global optimization methods. Hydrol Process 21:862–872

Zheng C, Wang P (1996) Parameter structure identification using tabu search and simulated annealing. Adv Water Resour 19:215–224

 DOI 10.1007/s10040-007-0228-3