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抽水源與污染釋放歷史鑑求

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中文摘要

地下水為天然的珍貴水資源，因此私人開發地下水受法律條文限制，不可違法取用。為了保護地下水資源，當某一地下水發現遭受擅自抽取，地下水抽水源的位置、抽水量、及抽水期間，即為需要探知的問題。藉由在監測井中，量測得的地下水位高度，以推求抽水源的問題，可稱為地下水抽水源鑑定問題。本研究將發展一個方法，包括模擬退火演算法(Simulated annealing)與 MODFLOW 模式，針對監測井中所量得的地下水水位，推求抽水源的位置、抽水量及抽取時間。為驗證所發展方法的正確性，先於某一地點，假設一抽水源及抽水量，並藉由 MODFLOW 計算各個監測井中的地下水水位，並將此水位視為其監測井中量測得的水頭值。隨後再利用所發展的方法，推求抽水源的位置、抽水量、及抽取時間。理論上，若模擬退火演算法所求得的最佳解，與真正抽水源的位置及抽水量相近時，則此時以 MODFLOW 所模擬的地下水洩降，應與量測水位洩降的誤差平方和為最小。

關鍵詞： 地下水、MODFLOW、抽水源鑑定、最佳化、模擬退火演算法

Abstract

Groundwater is a precious natural resource and it is not allowed to withdraw for private usage without governmental permission. In the real world, if the groundwater is detected to be used without any approval, the pumping source location, pumping rate, and pumping period are important information and needed to be identified. Locating the unknown source is an inverse problem and can be considered as a pumping source identification problem. An approach based on the simulated annealing (SA) and three-dimensional groundwater flow model (MODFLOW-2000) is developed to estimate the pumping source information. In order to verify the validity of the present approach, a pumping well is assumed to install at known location and withdraws the groundwater at a known pumping rate. After a specified time, the hydraulic head (hereafter called observed head) at observation wells can be simulated by MODFLOW. Then the proposed approach is chosen to estimate the pumping source information when minimizing the sum of square errors between the simulated heads and observed heads at the observed wells.

Keywords: Groundwater, MODFLOW, pumping source identification, optimization, simulated annealing

1. Introduction

Groundwater is a precious natural freshwater resource and has advantages of convenient availability near the point of use, excellent quality, and relatively low cost of development [*Todd and Mays*, 2005]. The groundwater resource usually is not allowed to pump for private use without governmental permit. Illegal pumping may have an adverse effect on the groundwater flow system, and moreover disturb the quality of the groundwater in a groundwater contamination site. An illegal pumping may change the groundwater flow pattern and agitate the capture zone at an ongoing remediation site. Thus, there is a need to develop a methodology for estimating the unknown pumping source information from a practical viewpoint.

Stochastic optimization methods such as genetic algorithms (GAs) and simulated annealing (SA) are the new global optimization methods. Differing from the gradient-type approaches, these global optimization methods are iteratively to renew the trial solution by the objective function value in determining the global optimum. The first advantage of these global optimization methods is that the user doesn't need much experience in providing the initial guesses for solving optimization problems. The initial guesses can be arbitrarily given or even generated by a random number generator, and still achieve optimal results. The second advantage is that these global optimization methods do not need the calculations for the derivates to renew the trial solution. The global optimization methods were successfully applied in wide range of optimization applications such as capacity extension for pipe network system [*Cunha and Sousa*, 1999; *Monem and Namdarian*, 2005], parameter calibration and identification problems [*Zheng and Wang*, 1996; *Cooper et al.*, 1997; *Li et al.*, 1999; *Guo and Zheng*, 2005; *Lin and Yeh*, 2005; *Yeh et al.*, 2006], groundwater management problems [*Dougherty and Marryott*, 1991; *Marryott et al.*, 1993], groundwater remediation system problems [*Kuo et al.*, 1992; *Marryott*, 1996; *Rizzo and Daugherty*, 1996; *Tung et al.*, 2003; *Shieh and Peralta*, 2005], and source identification of groundwater contamination problems. *Romeo and Sangiovanni-Vincentelli* [1991] used homogeneous and inhomogeneous Markov chain theories to prove that SA can converge to global optimal solutions. SA was an evolution from descent search method, but the major drawback of the descent method was the obtained solution might end up in a local optimum [*Rayward-Smith et al.*, 1996]. To avoid obtaining local optimum, the Metropolis mechanism controls which ascent moves could be accepted [*Rayward-Smith et al.*, 1996]. Therefore, the SA has a property of using descent strategy but allowing random ascent moves to avoid possible trap in a local optimum, preventing the SA from having the same problem as the descent method. In addition, *Shieh and Peralta* [2005] mentioned that the straightforward formulation, no requirement for computing derivatives, and easily implemented with ground water simulation models, are the main advantages as employed SA to solve the optimization problem.

The aim of this work is to develop an approach called SA-MF using SA incorporated with the numerical flow model, modular three-dimensional finite-difference ground-water flow model (or called MODFLOW-2000). The numerical approach can be used to estimate the pumping source information including the pumping source location, pumping rate, and pumping period in a groundwater flow system. A synthetic problem is designed test the validity of proposed approaches. The problem includes a hypothetic pumping well which is assumed at a specific location and withdraws the groundwater at a specified flow rate for a period of time. The temporal distribution of water level (hereafter called measured head) at the observation wells can be obtained from the MODFLOW-2000. In the pumping source information estimation process, SA is responsible for generating a series of trial solutions for the pumping source location, pumping rate, and pumping time. These trial solutions are then used as input in MODFLOW-2000 to calculate the simulated head distributions. The pumping source information can be siumlated by the proposed approach when minimizing the sum of square errors between the simulated heads and measured heads at the observation wells.

2. Methodology

(1) Groundwater flow model

The three-dimensional equation describing the groundwater flow can be expressed as [*Harbaugh and McDonald*, 1988]

$$\frac{\partial}{\partial x_i}\left(K_{ij} \frac{\partial h}{\partial x_i} \right) + W = S_s \frac{\partial h}{\partial t} \quad (1)$$

where h is the hydraulic head [L], K_{ij} is the hydraulic conductivity tensor [L/T], S_s is the specific storage [L^{-1}], W is the volumetric flux per unit volume representing sources and/or sink (negative for flow out and positive for flow in [L/T]), x_i are the Cartesian coordinates, and t is time [T].

Equation (1), together with specification of flow and/or head conditions at boundaries of an aquifer system and specification of initial head conditions, constitutes a mathematical model of a groundwater flow system. The computer model MODFLOW-2000 developed by the United State Geology Survey is used to simulate the head distribution for a given aquifer system. MODFLOW-2000 expends upon the modularization approach that was originally included in MODFLOW and simulates steady-state and transient flow in an irregularly shaped flow system with the aquifer being confined, unconfined, or a combination of confined and unconfined [*Harbaugh et al.*, 2000].

(2) SA-MF Implementation

Fig.1 demonstrates the schematic flowchart of SA-MF which includes six steps. The first step is to initialize the initial solution. All initial guesses are generated by random number generator within the solution domain. The solution domain for each unknown variable must be specified to confine the generated solutions being reasonable. The second and three steps are respectively to calculate the simulated heads by MODFLOW-2000 with the guess values and the objective function value (OFV) defined as

$$Minimize \ \ f = \frac{1}{nm \times nstep} \sum_{j=1}^{nstep} \sum_{i=1}^{nm} (h_{ij,sim} - h_{ij,mes})^2 \quad (2)$$

where $nstep$ is the number of the measured heads, nm is the number of observation wells, $h_{ij,sim}$ is the simulated head at jth time step at ith observation well, $h_{ij,mes}$ is the measured head at jth time step and at ith observation well. Now the initial solution is considered as the current optimal solution.

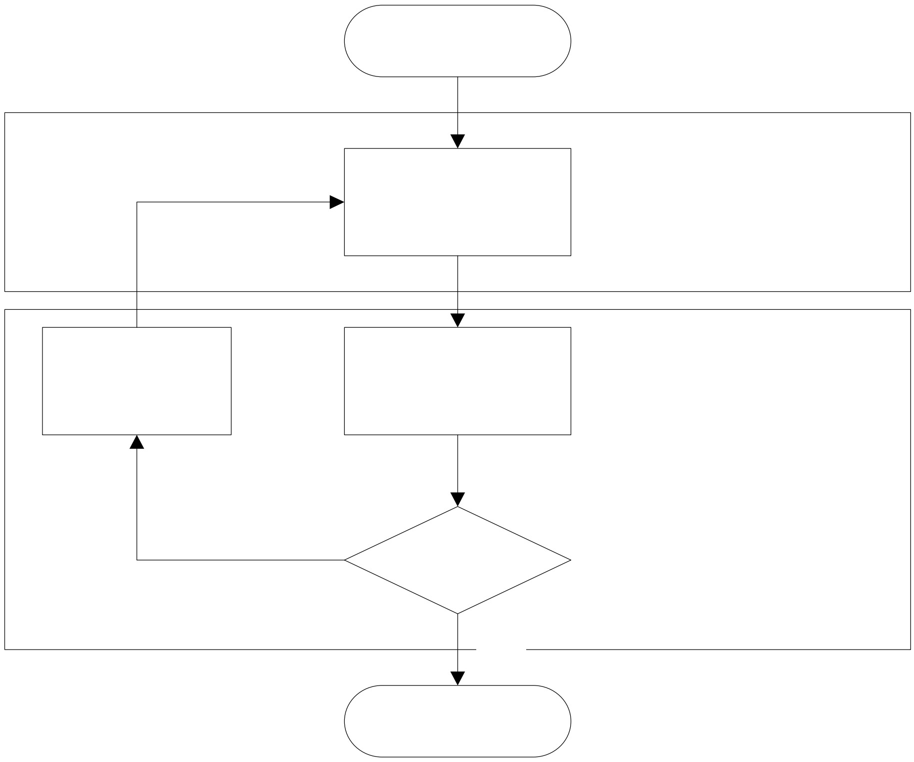

Figure 1 The schematic flowchart of SA-MF

The fourth step is to check the trial solution with the correspondent OFV to see whether this one is a new optimum or not. If the OFV of the trial solution is better than the current optimal solution or if the trial solution satisfies Metropolis's criterion, the current optimal solution is replaced by the trial solution in the sixth step. The Metropolis's criterion is given as [*Pham and Karaboga*, 2000]:

$$P_{SA} = \begin{cases} 1 & ,if \quad f(x') \le f(x) \\ \exp\left(\dfrac{f(x) - f(x')}{Te}\right) & ,if \quad f(x') > f(x) \end{cases} \qquad (3)$$

where P_{SA} is the acceptance probability of the trial solution, x and $f(x)$ are respectively the current optimal solution and its OFV. Similarly, x' and $f(x')$ are respectively the trial solution and the correspondent OFV, Te is a control parameter to analogy the temperature in physical world. Note that the initial guess is forthrightly set as the current optimum.

The fifth step is to check the obtained solution whether satisfies the stopping criteria or not. The stopping criterion is chosen as if the absolute difference between the two OFVs obtained at two consecutive temperatures is less than 10^{-6} four times successively. If the new trial solution meets the stopping criterion, the SA-MF is terminated. Otherwise, the algorithm will continue generating the new trial solution in the six step.

3. Synthetic homogeneous and isotropic unconfined aquifer

Four unknown variables: the source location of x and y coordinates, pumping rate, and pumping period are considered for solving the problem of pumping source information estimation. Note that SA-MF determines the source location right at the center of the finite difference grid. Four scenarios are considered in this study. Scenario 1 is designed to verify the minimum requirement on the number of measured heads for effectively solving the pumping source identification problem. The purpose of scenario 2 is to examine the influence of measurement error in drawdown on the estimated results. Scenario 3 is used to find an effective way to increase the identified accuracy as the measurement error level is high. Finally, the fourth scenario is to determine the requirement of the number of observation wells in pumping source identification.

(1) Site description

A hypothetical example is used to illustrate the pumping source identification procedure for a problem in a homogenous and isotropic confined aquifer. The aquifer length and width are both 1000 m and the aquifer thickness is 20 m. The top and bottom elevations, hydraulic conductivity, porosity, and storage coefficient are 10.0 and -10.0 m, 5×10^{-6} m/sec, 0.1, and 1×10^{-4}, respectively. The finite difference grids are block-centered and the related boundary conditions for the aquifer system are shown in figure 2. The upper and lower boundaries are specified as no flux boundaries and the left and right boundaries are specified as constant head boundaries. The elevations of the hydraulic head at left and right boundaries are 30.0 and 20.0 m, respectively. The grid width and length are both 10 m; thus, the number of finite difference meshes is 100 × 100. This example assumes that a pumping well P1 is located at (495 m, 495 m) and the pumping rate and pumping period are 200.0 CMD (m^3/day) and 60.0 minutes, respectively.

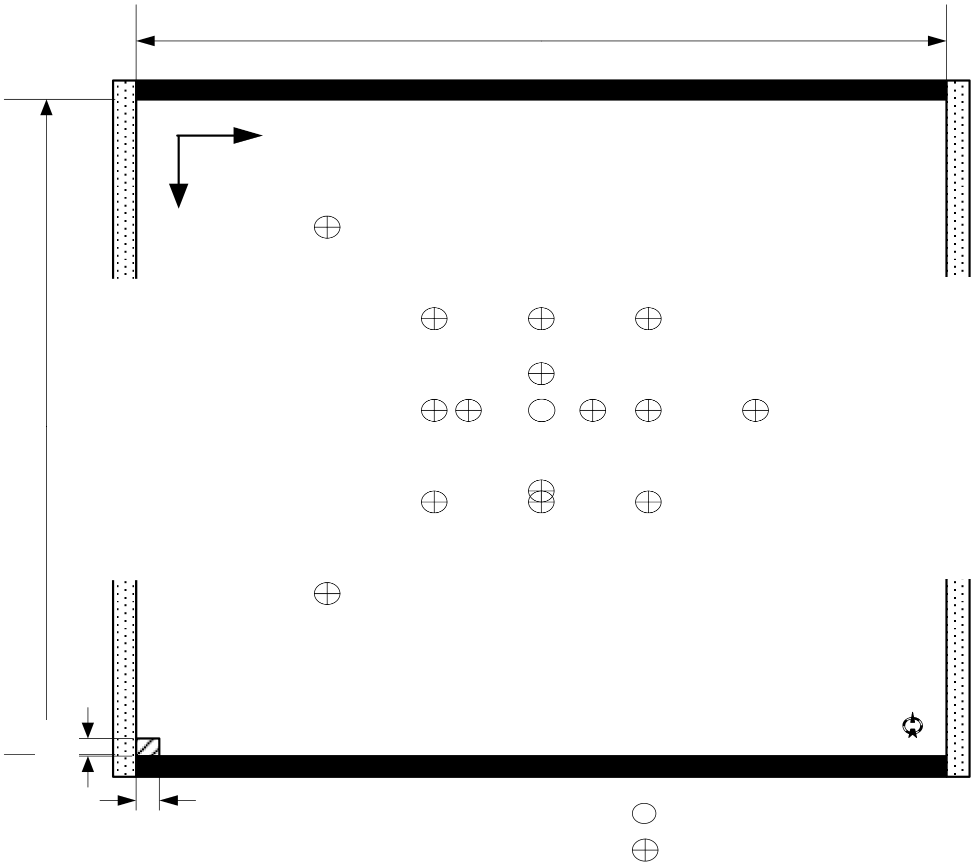

Figure 2 The plan view of hypothetic aquifer site

The measured heads at 15 observation wells indicated in Fig. 2 are simulated using MODFLOW-2000 and listed in Table 1. Notice that the drawdown at a distance of 500 m away from P1 is smaller than 0.001m when the pumping rate is 200 CMD and the pumping period is less than 170 minutes based on the calculation using Theis solution [*Todd and Mays*, 2005]. All the nodal points are considered as the suspicious pumping source locations except those meshes containing the observation wells. The upper bounds for the pumping rate and pumping period are set as 1000.0 CMD and 120.0 minutes, respectively, and the lower bounds are both zero. The *NS*, *NT*, initial temperature, and R_{Te} are chosen as 20, 10, 5, and 0.8, respectively. All initial guesses in the case studies are given by random number generator.

Table 1 The location and observed hydraulic head at observed wells for homogeneous and isotropic confined aquifer

Observation wells	Location	Measured heads(m)		
		Initial state	Pumping period	
			T = 30 (min)	T = 60 (min)
N-1	(465 m, 495 m)	25.041	22.621	21.275
N-2	(395 m, 495 m)	25.040	24.769	24.388
NW-1	(395 m, 395 m)	26.031	25.945	25.781
NW-2	(295 m, 295 m)	27.023	27.02	27.013
W-1	(495 m, 425 m)	25.734	25.086	24.408
W-2	(495 m, 395 m)	26.031	25.759	25.378
SW-1	(595 m, 395 m)	26.031	25.945	25.781
SW-2	(695 m, 295 m)	27.022	27.020	27.012
S-1	(585 m, 495 m)	25.040	24.680	24.216
S-2	(595 m, 495 m)	25.040	24.769	24.388
SE-1	(595 m, 595 m)	24.051	23.965	23.801
E-1	(495 m, 535 m)	24.645	22.958	21.809
E-2	(495 m, 595 m)	24.051	23.779	23.398
E-3	(495 m, 695 m)	23.062	23.043	22.995
NE-1	(395 m, 595 m)	24.050	23.964	23.800

4. Results and discussion

(1) Required number of measured heads

The purpose of this scenario is to explore the required number of measured heads in identifying the pumping source information in a homogeneous and isotropic aquifer site. Mathematically, at least four measured drawdowns are needed to solve those four unknowns. Eight cases are designed to investigate the influence of the number of measured drawdowns on the results of pumping source estimation. Four measured heads are used to estimate the pumping source information in cases 1-1 to 1-4 while five measured heads are used in cases 1-5 to 1-8. The analyzed results using four observations with different allocation of the observation wells are shown in Table 2. The estimated pumping locations are correctly determined at (495 m, 495 m) in cases 1-1, 1-2 and 1-4. Yet, the estimated location of (485 m, 505 m) in case 1-3 is incorrect. In cases 1-1, 1-2, and 1-4, the estimated pumping rates are respectively 200.99, 216.22, and 198.92 CMD and the estimated pumping periods are 54.22, 43.98, and 59.57 minutes, respectively. The largest relative errors are 8.11% in the estimated pumping rate and 26.7 % in the estimated pumping period in case 1-2.

While the number of measured heads is increased to five, the estimated source locations for cases 1-5 to 1-8 are all correct and the estimated pumping rates and pumping periods are all close to the correct solutions. The largest relative errors are -1.89% in the obtained pumping rate in case 1-7 and -2.3% in the estimated pumping period in case 1-5. Obviously, one more measured head is useful in estimating pumping source information. Thus, the number of measured heads is suggested to be more than one at least to the number of unknown variables when solving the pumping source identification problem.

Table 2 The required number of measured heads in determining the pumping source information

Case	Number of measured head	Observation wells	Identified results		
			Source location	Pumping rate (CMD)	Pumping period (min)
Pumping period is unknown					
1-1	4	N-1, W-1, S-1, E-1	(495 m, 495 m)	200.99	54.22
1-2		N-2, W-2, S-2, E-2	(495 m, 495 m)	216.22	43.98
1-3		NW-1, SW-1, SE-1, NE-1	(485 m, 505 m)	226.90	72.42
1-4		NW-2, SW-2, E-3, E-1	(495 m, 495 m)	198.92	59.57
1-5	5	N-1, W-1, S-1, S-2, E-1	(495 m, 495 m)	200.21	58.62
1-6		N-1, N-2, W-2, S-2, E-2	(495 m, 495 m)	198.73	60.02
1-7		NW-1, SW-1, SE-1, E-2, NE-1	(495 m, 495 m)	196.22	61.26
1-8		NW-2, SW-2, E-2, E-3, E-1	(495 m, 495 m)	198.99	60.38

(2) Effect of measurement error in hydraulic head

Scenario 2 considers that the measured head has error and the disturbed measured head is expressed as

$$h_{i,obs}^{'} = h_{i,obs} \times (1 + Er \times RD_3) \tag{4}$$

where $h'_{i,obs}$ is the disturbed measured head, *Er* is the level of measurement error, and RD_3 is a random standard normal deviate generated by the routine RNNOF of IMSL [2003]. Three different values of *Er*, i.e., 1 cm, 2 cm, and 3 cm, are chosen in this scenario and ten runs are performed for each level of measurement error. The average of estimated pumping rate and pumping period are respectively 199.42 CMD and 60.41 minutes. The largest relative errors are respectively -1.24 % in the estimated pumping rate and 3.72% in the estimated pumping period in case 2-2 as *Er* is 1 cm. In addition, the average of the estimated pumping rate and pumping period are respectively are 199.24 CMD and 60.64 minutes. The largest relative errors are respectively -2.84 % in the estimated pumping rate and 11.55% in the estimated pumping period in case 2-20 as *Er* is 2 cm. However, as the measurement error level increases to 3 cm, only seven out of ten runs obtain the correct source location as indicated in Table 3. The average of the estimated pumping rate and pumping period in those seven runs are respectively 199.97 CMD and 60.24 minutes. The largest relative errors are respectively 3.65% in the estimated pumping rate and -9.28% in estimated pumping rate in case 2-30 as *Er* is 3 cm.

Table 3 The identified results while the measurement contains error

Case	Identified results		
	Source location	Pumping rate (CMD)	Pumping period (min)
Maximum error = 1 cm			
2-1	(495 m, 495 m)	198.42	60.54
2-2	(495 m, 495 m)	197.53	62.23
2-3	(495 m, 495 m)	200.12	60.08
2-4	(495 m, 495 m)	199.43	60.12
2-5	(495 m, 495 m)	200.63	59.93
2-6	(495 m, 495 m)	198.12	61.12
2-7	(495 m, 495 m)	198.96	60.43
2-8	(495 m, 495 m)	200.72	59.21
2-9	(495 m, 495 m)	198.43	61.73
2-10	(495 m, 495 m)	201.87	58.75
Maximum error = 2 cm			
2-11	(495 m, 495 m)	197.32	61.21
2-12	(495 m, 495 m)	200.88	59.83
2-13	(495 m, 495 m)	201.32	58.76
2-14	(495 m, 495 m)	199.08	60.19
2-15	(495 m, 495 m)	203.43	56.42
2-16	(495 m, 495 m)	196.43	62.48
2-17	(495 m, 495 m)	197.83	62.13
2-18	(495 m, 495 m)	203.53	56.83
2-19	(495 m, 495 m)	198.21	61.63
2-20	(495 m, 495 m)	194.32	66.93
Maximum error = 3 cm			
2-21	(495 m, 495 m)	198.50	61.42
2-22	*(505 m, 505 m)*	*205.51*	*54.32*
2-23	(505 m, 505 m)	*199.23*	*60.45*
2-24	(495 m, 495 m)	202.67	58.48
2-25	*(495 m, 505 m)*	*200.68*	*60.43*
2-26	(495 m, 495 m)	204.13	55.46
2-27	(495 m, 495 m)	193.98	66.43
2-28	(495 m, 495 m)	194.15	64.98
2-29	*(505 m, 495 m)*	*203.12*	*62.30*
2-30	(495 m, 495 m)	207.13	54.43

(3) Improving the performance as measurement contains error

Based on the results obtained in scenario 2, the estimated pumping source location, pumping rate, and pumping period may be incorrect as the level of measurement error increases. Accordingly, cases 3-1 to 3-8 are designed to find an effective way to increase the accuracy of the identified result as the measurement error level is high. In cases 3-1 to 3-4, the measured heads are taken from five different observation wells. Cases 3-5 to 3-6 and cases 3-7 to 3-8 are respectively used six and seven measured heads to estimate the pumping information. All the measured heads are also considered to add the measurement error with the maximum value of *Er* is 3 cm. The estimated pumping source location, pumping rate, and pumping period are correct in cases 3-1 and 3-2. The accuracy of the results is decreased as the average distance from the observation wells is increased as indicated in cases 3-3 and 3-4. However, as the number of the measured heads increase to six or seven, the pumping source location, pumping rate, and pumping period are all correctly determined in cases 3-5 and 3-8 as indicated in Table 4. Therefore, if the level of measurement error is high, the best way to obtain good identified results is to employ more measured head data in the pumping source estimation.

Table 4 The effect between the identified result and the observation wells at different average distance with the maximum measurement error is 3 cm

Case	Observation wells	Average distance (m)	Identified results		
			Source location	Pumping rate (CMD)	Pumping period (min)
3-1	N-1, W-1, S-1, S-2, E-1	66.0	(495 m, 495 m)	198.50	61.42
3-2	N-1, N-2, W-2, S-2, E-2	86.0	(495 m, 495 m)	197.26	62.38
3-3	NW-1, SW-1, SW-2, SE-1, NE-1	169.7	*(505 m, 485 m)*	*195.18*	*64.29*
3-4	NW-2, SW-2, E-1, E-2, E-3	181.1	*(455 m, 545 m)*	*208.31*	*50.41*
3-5	NW-1, SW-1, S-2,SE-1, NE-1, E-2	120.5	(495 m, 495 m)	198.76	61.18
3-6	NW-2, SW-2, S-2 E-1, E-2, E-3,	150.9	(495 m, 495 m)	202.42	58.31
3-7	N-2, NW-1, SW-1, S-2,SE-1, NE-1, E-2	123.7	(495 m, 495 m)	199.15	60.73
3-8	N-2, NW-2, SW-2, S-2, E-1, E-2,E-3	157.9	(495 m, 495 m)	202.42	57.43

(4) Required number of observation wells

Twenty-three case studies in scenario 4 are designed to examine the effect of using the observations measured at two different time steps on the estimation for the pumping source information and the results are listed in Table 5. In cases 4-1 to 4-3, eight observations measured at four wells are used to determine the pumping information. While in cases 4-4 to 4-11, six observations measured at three wells and four observations measured at two wells in cases 4-12 to 4-23 are utilized. As the number of observation wells is four or three, the determined pumping source location and pumping rate are correct. However, when the number of observation wells is given as two, only eight out of 12 runs obtain the correct source location and pumping rate. When a well is pumped, water is removed from the aquifer and the hydraulic surface forms a conic shape called cone of depression. Since three points construct a plane, the number of observation wells should be three at least for estimating the pumping source information.

Table 5 The requirement of the number of observation wells in determining the pumping source information

Case	Number of observation wells	Observation wells	Identified results		
			Source location	Pumping rate (CMD)	Pumping period (min)
4-1	4	N-1, W-1, S-1, E-1	(495 m, 495 m)	202.18	57.43
4-2		N-2, W-2, S-2, E-2	(495 m, 495 m)	198.66	61.29
4-3		NW-2, SW-2, E-3, E-1	(495 m, 495 m)	198.38	60.81
4-4	3	W-1, S-1, E-2	(495 m, 495 m)	198.64	61.32
4-5		N-1, W-1, S-1	(495 m, 495 m)	198.62	61.63
4-6		N-1, E-2, S-1	(495 m, 495 m)	198.58	61.58
4-7		N-1, W-1, E-2	(495 m, 495 m)	198.45	61.42
4-8		N-2, S-2, E-2	(495 m, 495 m)	197.88	60.92
4-9		N-2, W-1, S-2	(495 m, 495 m)	198.45	61.35
4-10		W-1, S-2, E-2	(495 m, 495 m)	198.48	61.72
4-11		N-2, W-1, E-2	(495 m, 495 m)	197.85	60.67
4-12	2	W-1, E-2	*(565 m, 385 m)*	*216.79*	*50.48*
4-13		S-1, E-2	(495 m, 495 m)	198.36	60.93
4-14		N-1, E-2	(495 m, 495 m)	197.17	62.04
4-15		W-1, S-1	*(425 m, 415 m)*	*199.51*	*59.87*
4-16		N-1, W-1	(495 m, 495 m)	198.12	61.42
4-17		N-1, S-1	(495 m, 495 m)	199.63	60.59
4-18		N-2, S-2	*(495 m, 475 m)*	*203.43*	*58.46*
4-19		S-2, E-2	(495 m, 495 m)	198.18	61.32
4-20		W-1, S-2	*(565 m, 385 m)*	*216.67*	*50.14*
4-21		N-2, E-2	(495 m, 495 m)	198.42	60.68
4-22		N-2, W-2	(495 m, 495 m)	198.32	61.32
4-23		W-1, E-2	(495 m, 495 m)	197.43	62.43

5. Concluding remarks

A new approach, SA-MF, is developed based on a three-dimensional groundwater flow, MODFLOW-2000, and SA for solving the pumping source identification problem. The SA is first employed to randomly generate the trial solutions, i.e., pumping source location, pumping rate, and pumping period and then the MODFLOW-2000 is employed to simulate the hydraulic heads at the observation wells. Four scenarios are designed to test the performance of SA-MF on the homogeneous, heterogeneous aquifer systems. Four conclusions can be drawn as follows.

First, the approach we developed is capable for estimating the pumping source information for problems in synthetic homogeneous aquifer and the estimations give good results. Second, the investigator does not need any experience to give reasonable initial guesses for the source information. The proposed approach can obtain good results even the initial guesses are generated by the random number generator. Third, five measured heads at least should be used to analyze the pumping source estimation problem and, at least three observation wells are required for effectively identifying the pumping source location, pumping rate, and pumping period. Fourth, if the level of measurement error is high, increasing the number of measured heads is the best way to estimate the pumping source information correctively and effectively. Thus, the important key for successfully estimating the pumping source information is to use more head observations.

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