

SOLUTION OF RELEASE HISTORY RECOVERY PROBLEMS OF GROUNDWATER POLLUTION SOURCES USING HARMONY SEARCH OPTIMIZATION ALGORITHM

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ABSTRACT

Groundwater contamination may originate from point and non-point sources. The major point and non-point sources are the leaking from the underground storage tanks, waste disposal sites, manufacturing facilities, and agricultural activities, etc. Note that contamination process of groundwater systems results with a pollution plume no matter where the contamination starts. This plume transports through subsurface based on the advection and hydrodynamic dispersion. To control the spreading process of this plume through longitudinal and transverse directions, the identification of its release history is a required task. In this paper, a new solution model is proposed for solving the release history recovery problems of the pollution sources in groundwater systems. In the proposed solution model, groundwater flow and transport processes have been simulated through MODFLOW and MT3DMS models, which are widely used solution models in groundwater modeling. These models are then integrated to an optimization model in which recently proposed heuristic harmony search (HS) optimization algorithm is used. The performance of the proposed solution model is compared to previously developed artificial neural networks (ANN) and genetic algorithm (GA) based solution models for error-free and measurement error conditions. The identified results indicate that the proposed solution model provides better results than both ANN and GA based solution models even if the measured pollution concentrations include high measurement errors.

1 INTRODUCTION

Release history recovery of the groundwater pollution sources is an important problem in groundwater modeling since these histories are the main system inputs of the management studies. If no information is available dealing with these release histories, the developed remediation strategies may not be successful for cleaning up the aquifer systems. Therefore, it is essential to recover the release histories of the potential pollution sources before starting the remediation studies.

The current literature includes many studies dealing with the pollution source identification problems in groundwater systems. The state-of-the-art and overview of the various solution approaches of pollution source identification problems are given in Atmadja and Bagtzoglou (2001), Michalak and Kitanidis (2004), Bagtzoglou and

Atmadja (2005). Among the proposed solution approaches, optimization approach is one of the most widely used solution approaches to solve the problem (Ayvaz, 2010a). The main idea of the optimization approaches is to generate the model inputs of the simulation model (i.e. flow and transport process) to best represent the recorded data which were collected from the observation locations.

It should be noted that although traditional non-heuristic optimization algorithms have been successively applied to the solution of pollution source identification problems, the quality of the identified solutions is dependent to the gradient of the objective function and initial solutions (Ayvaz, 2009). If taking the gradient of objective function is not possible and/or specified initial solutions are not well, obtaining the optimum solution through the non-heuristic optimization algorithms may not be possible. Therefore, heuristic optimization algorithms are usually preferred to apply to the solution of the optimization problems dealing with groundwater modeling. The major benefit of using heuristic algorithms is their ability of finding solutions without requiring gradients and special initial solutions (Ayvaz, 2009).

Recently, Geem et al. (2001) developed a new heuristic optimization algorithm, harmony search (HS), to solve engineering optimization problems. HS gets its inspiration from the musical improvisation process while most of the other heuristic algorithms mimic the natural events. It is well known that the purpose of the musical processes is to seek a musically pleased harmony through making several improvisations (Yang, 2009). This process is analogous to optimization process since the optimization aims to find the global optima by making several iterations. The main advantage of HS is that it does not require complex calculus, and therefore, solution of engineering problems through HS is easy (Ayvaz, 2007).

The main objective of this study is to propose a solution model that solves the release history recovery problem of the pollution sources in groundwater systems. In the proposed solution model, groundwater flow and pollution transport processes have been simulated through MODFLOW (McDonald and Harbough, 1988) and MT3DMS (Zheng and Wang, 1999) models. These solution models are then linked to HS based optimization model. The optimization model aims to determine the release histories by maximizing an objective function which is the modified coefficient of efficiency (E) between the observed and simulated concentration values at selected observation locations and times. The performance of the proposed S/O model is tested on a hypothetical aquifer model which was previously solved using artificial neural networks (ANN) (Singh et al., 2004) and genetic algorithm (GA) (Singh and Datta, 2006) based solution models. The results indicate that the proposed solution model well determines the release histories of the sources than both ANN and GA although the measured concentration values are corrupted with high measurement errors.

2 HARMONY SEARCH OPTIMIZATION ALGORITHM

Like other heuristic optimization algorithms, the HS is also inspired from a heuristic event. However, its main difference from the others is that HS does not get its main philosophy from a natural process, instead, gets from the musical improvisation which occurs when a group of musicians searches for a better state of harmony (Ayvaz, 2010b). This philosophy is first adapted to the solution of optimization problems by Geem et al. (2001). In this adaptation, each musician mimics to a decision variable and

the notes in the musicians' memories correspond to the values of the decision variables. When the musicians find the fantastic harmony from their memories, it means, a global optimum solution is obtained using the corresponding decision variables. Note that an aesthetic harmony may be improvised based on the following three operations (Ayvaz, 2010b):

- Playing a note from the harmony memory,
- Playing a note randomly from the possible note range,
- Playing a note which is close to another one stored in memory.

These operations are all musically based and integration of them allows finding a musically pleasing harmony. Adaptation of these musical operations into the engineering optimization problems is as follows:

- New variable values are selected from the harmony memory,
- New variable values are randomly selected from the possible random range,
- New variable values are further replaced with other values which are close to the current values.

Combination of these three operations allows searching a global optimum solution in an optimization framework. For continuous decision variables, the computational scheme of HS can be given as follows (Wikipedia, 2011):

1. Initialize the harmony memory: Generate initial solution vectors as many as HMS, $\mathbf{x}^1 \dots \mathbf{x}^{HMS}$.
2. Generate a new solution vector $\mathbf{x}'$ for each x'_i :
 - with probability HMCR select x'_i from memory, $x'_i = x_i^{Rnd(1, HMS)}$
3. Pitch adjustment: For each x'_i :
 - with probability PAR change x'_i as, $x'_i = x'_i \pm bw \times Rnd(0;1)$.
 - with probability (1-PAR) do nothing.
 - with probability (1-HMCR) select a new random value from the possible range.
4. If $\mathbf{x}'$ is better than the worst $\mathbf{x}^j$ in harmony memory, replace $\mathbf{x}^j$ with $\mathbf{x}'$.
5. Repeat step 2 to 5 until the given termination criterion is satisfied.

The solution parameters of HS are: Harmony Memory Size (HMS), Harmony Memory Considering Rate (HMCR), Pitch Adjusting Rate (PAR), and distance bandwidth (bw). Note that the HM is a matrix where the decision variables and the corresponding objective function values are stored. The HMCR and PAR parameters are used to improve the solution vector globally and locally. The computational procedure of HS is described in Figure 1.

As can be seen from Figure 1, each musician has several notes in their HM. The main question to be asked here is the "which notes will be played by the musicians to find a musically pleasing harmony?". Depending on the three operations of improvising a new harmony, the answer of this question is given as follows:

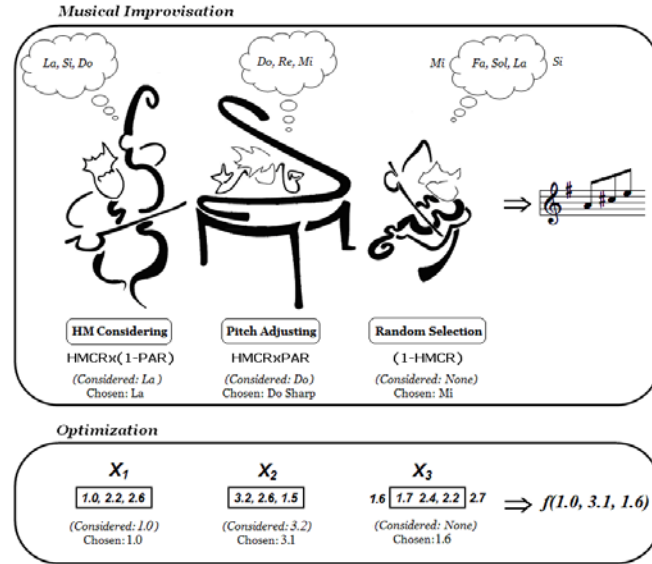


Figure 1. Analogy between musical improvisation and optimization (Ayvaz, 2010b)

Memory Consideration: The first musician in Figure 1 has three notes, {La, Si, Do} in his HM. With probability $HMCR \times (1-PAR)$, he decides to choose and play {La} from his HM. Since {La, Si, Do} corresponds to {1.0, 2.2, 2.6} in the optimization process, choosing and playing {La} corresponds to choosing and using {1.0} as the first decision variable.

Pitch Adjusting: The second musician in Figure 1 has also three notes, {Do, Re, Mi} in his HM. Unlike the first musician, with probability $HMCR \times PAR$, he chooses {Do} and plays its neighbor {Do#}. Since {Do} corresponds to {3.2} in the optimization process, its neighbor {Do#} corresponds to {3.1} which is a small random amount neighbor to {3.2}.

Random Selection: The third musician in Figure 1 has also three notes, {Fa, Sol, La} in his HM. Although his HM is used in the previous improvisations, due to his musical knowledge, he knows all the possible notes in the La Scale. Thus, he decides to choose and play a note randomly, for example {Mi} in this case. As differently from the possible data set stored in HM, {1.6} is randomly chosen and used in this case, even if it doesn't exist in HM.

After musicians' decision of what to play based on the memory consideration, pitch adjusting and random selection, the new harmony is composed as {La, Do#, Mi} which corresponds to {1.0, 3.1, 1.6} in the optimization process. This iterative process is repeated until the given termination criterion is satisfied. The detailed information about HS algorithm can be found at algorithm's web site at <http://www.hydroteq.com>.

3 MODEL DEVELOPMENT

As indicated in the previous sections, the main goal of this study is to develop a solution model that solves the release history recovery problem for groundwater

pollution sources. In the proposed solution model, only point sources are taken into account and it is assumed that these sources release a typical conservative pollutant at a uniform rate during the considered activity periods. In what follows, after giving the mathematical structure of simulation model, how this model is integrated to the HS based optimization model is described.

3.1 Simulation Model

Simulation model is one of the most important parts of the proposed solution model since it transforms the output of the optimization model into pollution concentrations at selected observation locations and time. Note that the calculation of pollution concentration at selected locations and time requires of knowing the hydraulic head distribution. Therefore, solution of groundwater flow equation is needed before solving the pollution transport equation. The governing partial differential equations for the steady-state flow and transient transport processes in a two dimensional aquifer system can be given as follows (Singh and Datta, 2006):

$$\frac{\partial}{\partial x_i} \left(T_{ij} \frac{\partial h}{\partial x_j} \right) = W \quad i, j = 1, 2 \quad (1)$$

$$\frac{\partial (bC)}{\partial t} = \frac{\partial}{\partial x_i} \left(bD_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (bCv_i) + \frac{C_s W}{\theta} \quad i, j = 1, 2 \quad (2)$$

where x_i and x_j are the Cartesian coordinates for $i, j = 1, 2$ [L], h is the hydraulic head [L], W is the volumetric flux per unit area [LT^{-1}], T_{ij} is the transmissivity tensor [L^2T^{-1}] which equals to $K_{ij}b$ where K_{ij} is the hydraulic conductivity tensor [LT^{-1}] and b is the saturated thickness of the aquifer [L], t is the time [T], C is the dissolved concentration [ML^{-3}], v_i is the seepage velocity [LT^{-1}], θ is the effective porosity [-], C_s is the dissolved concentration in a source or sink flux [ML^{-3}], D_{ij} is the hydrodynamic dispersion tensor [L^2T^{-1}] whose elements are calculated using the longitudinal (α_L) and transverse (α_T) dispersivities [L], molecular diffusion coefficient (D^*) [L^2T^{-1}], and v_i . Note that Equation (1) and (2) are related with each other through Darcy's Law as follows:

$$v_i = \frac{q_i}{\theta} = -\frac{K_{ij}}{\theta} \frac{\partial h}{\partial x_j} \quad i, j = 1, 2 \quad (3)$$

where q_i is the Darcy flux [LT^{-1}]. As indicated in the previous section, MODFLOW and MT3DMS models have been used to simulate the flow and transport processes defined in Equations (1) and (2).

3.2 Problem Formulation and Search Procedure

The problem of release history recovery has been solved based on HS based optimization model in this study. The main objective of the optimization model is to

maximize the efficiency between the simulated and measured pollution concentrations at selected observation well locations and time. With this purpose, the modified coefficient of efficiency (E) is used as the objective function. Note that the value of E varies from $-\infty$ to 1. An efficiency of 1 corresponds to a perfect match between the simulated and measured concentrations. The decision variables of the optimization model are the source flux terms ($\mathbf{q}$) which are the product of the liquid volume disposal rate and the pollution concentration in the sources (C_s). Mathematically, the optimization problem of release history recovery of groundwater pollution sources can be stated as follows (Ayvaz, 2010a):

$$E = \max \left(1 - \frac{\sum_{t=1}^{N_T} \sum_{k=1}^{N_d} |C_k(t) - \hat{C}_k(t)|}{\sum_{t=1}^{N_T} \sum_{k=1}^{N_d} |\hat{C}_k(t) - \bar{C}|} \right) \quad (4)$$

subject to

$$\mathbf{C} = f(\mathbf{q}) \quad (5)$$

$$\mathbf{q}_{\min} \leq \mathbf{q} \leq \mathbf{q}_{\max} \quad (6)$$

$$E + C_k(t) - 1 = \hat{C}_k(t) \quad k = 1, 2, 3, \dots, N_d; \quad t = 1, 2, 3, \dots, N_T \quad (7)$$

where N_T is the number of stress periods, N_d is the number of monitoring well locations, $C_k(t)$ is the simulated concentration at monitoring well location k and stress period t , $\hat{C}_k(t)$ is the measured concentration at monitoring well location k and stress period t , $\bar{C}$ is the average of measured concentrations, $\mathbf{C}$ is the vector of simulated concentrations, $\mathbf{q}$ is the vector of source fluxes such that $\mathbf{q} = [q_1, q_2, q_3, \dots, q_n]^T$, n is the number of sources to be identified, $f(\mathbf{q})$ is the simulation model which transforms the $\mathbf{q}$ into $\mathbf{C}$, $\mathbf{q}_{\min}$ and $\mathbf{q}_{\max}$ are the lower and upper bounds of the source fluxes.

3.3 Incorporating Measurement Errors

In this study, the performance of the proposed solution model is also evaluated for measurement error conditions. This is a required task since most of the field and laboratory studies result with erroneous measurements. With this purpose, all the measured concentrations are usually perturbed with error terms with normal distribution (Singh and Datta, 2006). Note that all the measured concentrations are hypothetically generated using the simulation model before starting the optimization model in this study. The perturbed pollution concentrations are computed as follows (Mahar and Datta, 2001):

$$\hat{\mathbf{C}} = \mathbf{C} + \mathbf{C} \mathbf{a} \cdot \quad (8)$$

where $\mathbf{\varepsilon}$ is an error matrix which includes the normally distributed error terms with zero mean and 1 standard deviation and a is a fraction such that $0 \leq a \leq 1$. According to Singh and Datta (2006), the value of a varies from 0.05 to 0.2. $a < 0.10$, $0.10 \leq a \leq 0.15$, and $a > 0.15$ correspond to low, moderate, and high noise levels, respectively.

It should be noted that Equation (8) provides one set of perturbed concentrations and this set corresponds to one sample realization. However, it is required to test the robustness of the proposed solution model for different sample realizations. With this purpose, measured concentration values are perturbed with different error terms and the problem is then solved for those perturbed values. After obtaining results for different sample realizations, the average values of the identified results are used to test the model performance. Note that 10 different realizations have been generated in this study to compare results with those obtained by ANN (Singh et al., 2004) and GA (Singh and Datta, 2006) based solution models.

3.4 Performance Evaluation

As indicated in the previous sections, the performance of the proposed solution model is tested on a hypothetical aquifer model for different measurement error conditions. The evaluation and comparison of the identified results are performed based on the normalized error (NE), percent average estimation error (PAEE), and standard deviation (SD). The NE can be defined as follows (Mahar and Datta, 2001):

$$NE = \frac{\sum_{t=1}^{N_T} \sum_{i=1}^n |\bar{q}_i(t) - \hat{q}_i(t)|}{\sum_{t=1}^{N_T} \sum_{i=1}^n \hat{q}_i(t)} \times 100 \quad (9)$$

where $\bar{q}_i(t)$ is the average of the identified source fluxes for the stress period t and source i , $\hat{q}_i(t)$ is the actual source flux for the stress period t and source i . Note that NE values are calculated by setting the number of realizations into 1 for error-free measurement condition. In such a case, $\bar{q}_i(t)$ equals to the identified source flux.

For each source flux term, the value of PAEE is calculated as follows (Mahar and Datta, 2001):

$$PAEE = \frac{|\bar{q}_i(t) - \hat{q}_i(t)|}{\hat{q}_i(t)} \times 100 \quad i = 1, 2, 3, \dots, n; \quad t = 1, 2, 3, \dots, N_T \quad (10)$$

Furthermore, accuracy of different realizations has been evaluated using SD value as follows:

$$SD = \sqrt{\frac{\sum_{r=1}^{N_R} (\tilde{q}_{i,r}(t) - \bar{q}_i(t))^2}{N_R - 1}} \quad i = 1, 2, 3, \dots, n; \quad t = 1, 2, 3, \dots, N_T \quad (11)$$

In Equation (11), $\tilde{q}_{i,r}(t)$ represents the estimated source flux for the stress period t ,

source i , and realization r , and N_R represents the number of realizations (e.g. 10 for this study).

4 NUMERICAL APPLICATION

The performance of the proposed solution model is evaluated on a well known aquifer model in literature. This aquifer model was previously solved through ANN (Singh et al., 2004) and GA (Singh and Datta, 2006) based solution models. Groundwater system has steady-state flow and unsteady-state transport conditions. It is assumed that the numbers, locations, and release periods are known and the main objective is to recover the release histories (source fluxes) of the potential sources. Figure 2 shows the hypothetical aquifer model under consideration.

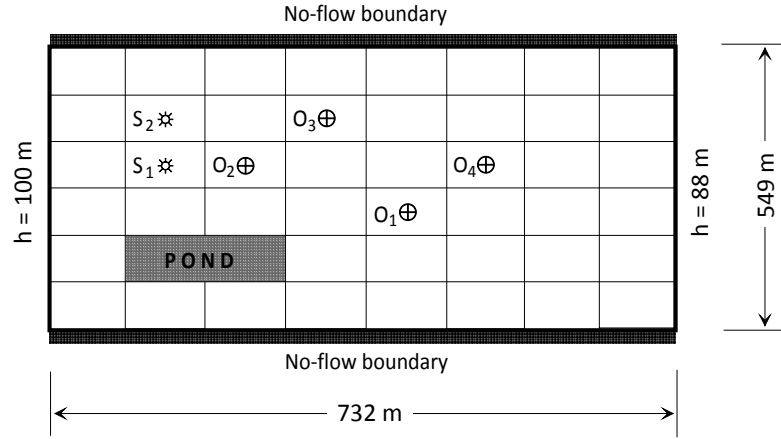


Figure 2. Hypothetical aquifer model under consideration

As can be seen from Figure 2, the aquifer has specified head boundary conditions on the west ($h = 100 \text{ m}$) and east ($h = 88 \text{ m}$), and no-flow at the other sides. Aquifer has 2 pollution sources ($S_1 - S_2$) and 4 monitoring wells ($O_1 - O_4$) where pollution concentrations are collected at the end of each activity periods. The initial concentration and concentration in the recharge from the pond is assumed to be zero. The total simulation time is 10 years and this time domain is equally divided into 40 stress periods. It is assumed that the both sources release a typical conservative contaminant with different rates through the first 5 years of the time domain. Table 1 and 2 give the related solution parameters and the actual values of the source fluxes for each year.

As can be seen from Table 2, S_1 is the active source and all the source fluxes of S_2 is zero. The number of decision variables (e.g. source fluxes in Table 2) is 10. The main goal of the optimization model is to maximize the efficiency between the simulated and measured concentration values at observation well locations by optimizing the source fluxes in Table 2. Since there are 4 observation wells and 40 stress periods, the total number of pollution observations to be used in the optimization model is 160. Note that all the observations are artificially simulated using MT3DMS model using the solution parameters given in Table 1 and 2.

Table 1. Related solution parameters

Parameters	Values
Hydraulic conductivity in x direction, K_{xx} (m/s)	0.0001
Hydraulic conductivity in y direction, K_{yy} (m/s)	0.0001
Effective porosity, θ	0.20
Longitudinal dispersion, α_L (m)	30.5
Transverse dispersion, α_T (m)	12.2
Aquifer thickness, b (m)	30.5
Grid spacing in x direction, Δx (m)	91.5
Grid spacing in y direction, Δy (m)	91.5
Length of stress periods, Δt ($months$)	3
Recharge from the pond, q_r (m/s) ^a	2.15

^a Amount of clean water recharge from the pond

Table 2. Actual values of the source fluxes

Pollution Sources	Source Fluxes at each stress period (g/s)				
	Year 1	Year 2	Year 3	Year 4	Year 5
S_1	48.8	0.0	10.0	42.0	36.0
S_2	0.0	0.0	0.0	0.0	0.0

Figure 3 shows the artificially simulated concentrations at the end of each stress period for both error-free and measurement error conditions ($a = 0.10$).

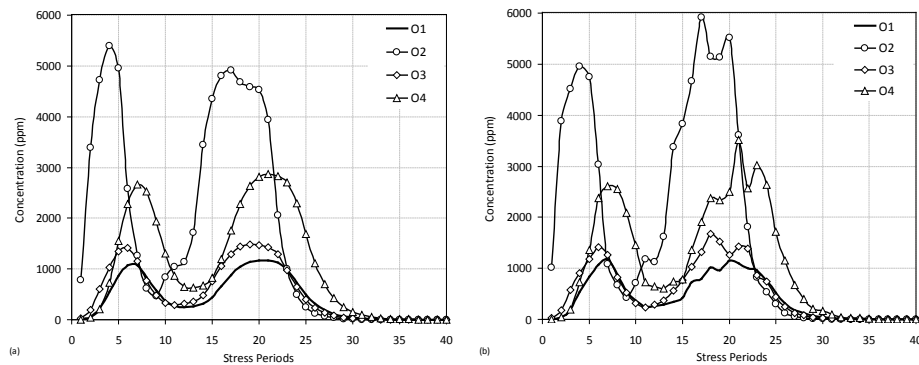


Figure 3. Artificially simulated pollution concentrations at the observation well locations (a): Error-free condition; (b): Measurement error condition for $a = 0.10$

Using the pollution observations given in Figure 3, the release history recovery problem can be solved using the proposed solution model. Note that the related solution parameters of HS are set as: HMS = 10, HMCR = 0.95, PAR = 0.50. These values are all empirically based and recommended by Lee et al. (2005). Giving the maximum

number of simulations as the termination criterion, the global search process is ended at the end of 10,000th simulations. Note that bounds of the source fluxes are fixed to $\tilde{q}_{\min} = 0$ and $\tilde{q}_{\max} = 100 \text{ g/s}$. Using this solution parameter set, the comparison of the identified source fluxes with those obtained by using ANN and GA based solution models for error-free and measurement error conditions ($a = 0.10$) can be seen in Figure 4.

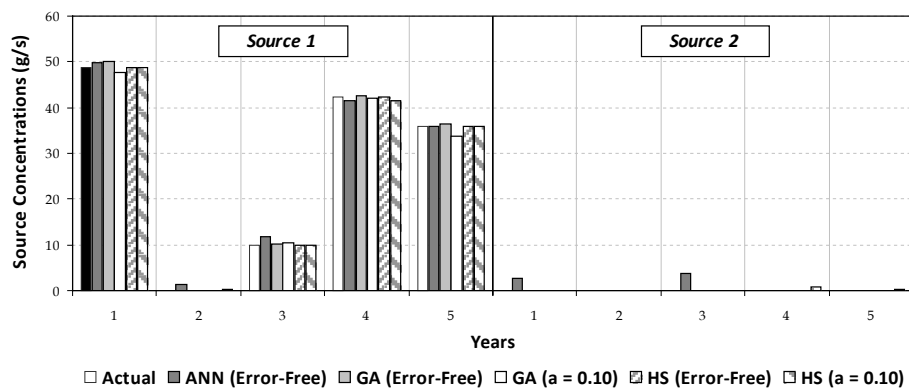


Figure 4. Comparison of the identified source fluxes with ANN (Singh et al., 2004) and GA (Singh and Datta, 2006)

As can be seen from Figure 4, the identified source fluxes well agree with the actual values than both ANN and GA. For different size of noise levels, comparison of the identified results with those obtained using the ANN and GA are shown in Table 3.

Table 3. Comparison of the identified results with ANN (Singh et al., 2004) and GA (Singh and Datta, 2006) for different noise levels

Noise Levels (a)	ANN (Singh et al., 2004)	GA (Singh and Datta, 2006)	HS		
	NE (%)	NE (%)	NE (%)	E	Number of Simulations
0.00	8.11	2.33	0.17 ^a	0.9994	4,683
0.05	8.70	2.33	0.74 ^b	0.9584 ^c	7,493
0.10	9.83	2.53	1.48 ^b	0.9170 ^c	8,864
0.15	11.29	4.96	2.65 ^b	0.8760 ^c	6,961
0.20	12.83	8.38	3.19 ^b	0.8360 ^c	7,929

^a $N_R = 1$

^b $N_R = 10$

^c Average of 10 sample realizations.

As can be seen from Table 3, increase in the noise level leads to increase NE and decrease the final objective function values. Comparison of the identified results indicates that the proposed solution model provides better NE values than ANN and GA based solution models for all the noise levels. For $a = 0.10$, Table 4 lists the average identified source fluxes and the final PAEE and SD values.

Table 4. Comparison of the identified and actual source fluxes and final values of the PAEE and SD for $\alpha = 0.10$

Year	Source Number	Actual Source Flux	Estimated Source Fluxes		
			Average of 10 Realizations	PAEE	SD
1	S_1	48.8	48.81	0.01	0.73
2	S_1	0	0.14	N/A	0.23
3	S_1	10	9.84	1.64	0.40
4	S_1	42	41.62	0.90	2.46
5	S_1	36	35.99	0.03	1.58
1	S_2	0	0.10	N/A	0.22
2	S_2	0	0.06	N/A	0.17
3	S_2	0	0.11	N/A	0.27
4	S_2	0	0.79	N/A	1.13
5	S_2	0	0.27	N/A	0.51

As can be seen from Table 4, average source fluxes of 10 sample realizations well agree with the actual values. For this noise level, maximum PAEE and SD values are 1.64 and 2.46, respectively. Note that the GA based solution model of Singh and Datta (2006) obtained the maximum value of PAEE and SD as 3.17 and 1.41, respectively. It is concluded that the proposed solution model provides better results than GA in terms of maximum PAEE and SD values.

5 CONCLUSIONS

In this study, a solution model has been proposed for solving the release history recovery problem of groundwater pollution sources. In the proposed solution model, MODFLOW and MT3DMS models are used to simulate the flow and transport processes in groundwater system. These models are then linked to a HS based optimization model. The main objective of HS based optimization model is to determine the unknown source fluxes by maximizing the modified coefficient of efficiency which is calculated between the measured and simulated pollution concentrations at selected observation well locations and time. In order to evaluate the performance of the proposed solution model, the problem is solved on a previously solved aquifer model through ANN and GA solution approaches for both error-free and measurement error conditions. The identified results indicate that the proposed model provides better results than ANN and GA in terms of the final values of NE, PAEE and SD measures.

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