International Journal of Engineering Research
Volume No.7, Issue Special 4, pp : 394-397

ISSN:2319-6890 (online),2347-5013(print)
9,10 March 2018

Optimal Identification of Groundwater Pollution Sources

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Abstract: An inverse problem model of groundwater pollution source identification has been presented in the present study. The model is based upon linked simulation optimization approach and invokes a finite difference based simulator and an Exhaustive Search based optimizer. The model estimated pollution source characteristics are those set of source characteristics which provide the closest match between observed and the simulated concentration field. The pollution source characteristics include number of sources, their locations and release flux rates. Finding the optimum number of sources and their location is an advantage of this model, since most of the source identification problem involves a priori known potential location. The model has been illustrated for a hypothetical study area, with known flow/transport boundary conditions and flow/transport parameters. Two dimensional steady state flow and transient transport has been considered. Identified results indicated that the proposed methodology can be used to solve the inverse problem of groundwater pollution source identification.

Keywords : **Groundwater Pollution Sources,** linked simulation optimization

1. *Introduction*

Groundwater source identification is an important problem in groundwater risk assessment studies and groundwater management problems. It is a type of an inverse problem in context of groundwater solute transport modelling. In this inverse problem source characteristics are obtained for a given set of concentration and head fields and flow and transport parameters.

Several methods have been reported to solve the source identification inverse problem. These methods can be broadly classified as Deterministic direct methods (Skaggs and Kabala 1994, 1995, 1998; Sidauruk et. al. 1997; Ball et al. 1997; Liu and Ball 1999; Atmadja and Bagtzoglou 2001), Probabilistic and Geostatistical simulation approaches (Bagtzoglou et al. 1991, 1992; Snodgrass and Kitanidis 1997; Michalak and Kitanidis 2010; Woodbury and Ulyrich 1993, 1996, 1998) and Indirect approaches such as Optimization approaches (Gorelick 1982, 1983; Mahar and Dutta 2000, 2001; Aral et al. 2001; Singh et al. 2004; Singh and Datta 2006; Datta et al. 2009; Ayvaz 2010; Jha and Dutta 2013, 2015; Chaubey and Kashyap 2014, 2017). Detailed review of studies related to source identification problem has been performed by Atmadja and Bagtzoglou (2001) and Amirabdollahian and Datta (2013).

Optimization is one of the most common solution approaches for source identification problem. Optimization approach consists of the integration of simulation with the optimization model. Depending upon the incorporation of Simulation model into the optimization model it can be termed as embedded method i.e. incorporating simulation model as constraints (Mahar and Dutta 2000, 2001), Kernel method i.e. incorporating simulation model as as concentration response matrix (Gorelick 1982, 1983) and Linked Simulation optimization approach i.e. linking simulation model externally with an optimization model (Datta et al. 2009, Aral et al. 2001, Singh et al. 2004, Singh and Datta 2006, Ayvaz 2010, Jha and Dutta 2013, 2015, Chaubey and Kashyap 2014, 2017).

Simulation model solves the governing flow and solute transport equation for a given initial and boundary conditions, flow and transport parameters. It is integrated with the optimization model which aims at selecting that set of sources characteristics (location, magnitude and release history) which results in simulated concentrations closest with the local groundwater solute concentration data.

Present study is based on the linked simulation optimization (LSO) approach for groundwater pollution source identification. Source characteristics usually involve source location, strength and release history. In most of the studies related to groundwater pollution source identification, source number and location is known a priori. An attempt has been made by Ayvaz (2010) in solving the inverse problem with unknown number of sources and their location by considering a hypothetical example.

Present study is an extended work of Chaubey and Kashyap (2014). In latter work source locations were assigned a priori and then the source strength was determined. Source characteristics in the present context comprise number of sources, their location and their fluxes. The model invokes a finite difference based simulator and an Exhaustive Search based optimizer.

2. Methodology

Simulation model based on governing 2D steady state groundwater solute transport equation is used. It can be given as (Bear, 1979)

$$\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial x}\left(D_{yy}\frac{\partial C}{\partial y}\right)-\frac{\partial}{\partial x}(uC)-\frac{\partial}{\partial y}(vC)+\frac{W}{b\varphi}=0 \quad (1)$$

where, D_{xx} and D_{yy} = hydrodynamic dispersion coefficients, u and v = seepage velocities along x and y direction respectively, W = pollution source flux, b = aquifer thickness, φ = effective porosity of the aquifer, C = concentration of solute dissolved in groundwater. The velocities in Eq. 1 are given by,

$$u=\frac{\frac{\partial h}{\partial x}T_{xx}}{b*\varphi}\text{and}v=\frac{\frac{\partial h}{\partial y}T_{yy}}{b*\varphi} \quad (2)$$

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where, h = nodal head, T_{xx} and T_{yy} = transmissivities in x and y direction respectively.

Hydrodynamic dispersion coefficients are taken as $D_{xx} = \alpha_L|u|$ and $D_{yy} = \alpha_T|v|$ where, α_L = longitudinal dispersivity and α_T = transverse dispersivity.

The necessary head fields for computing velocity vector are simulated by solving following two dimensional, steady state groundwater flow equation (Bear, 1979):

$$\frac{\partial}{\partial x}\left(T_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_{yy}\frac{\partial h}{\partial y}\right) - W' = 0 \qquad (3)$$

where, x and y = cartesian coordinates in the directions of principal permeability and W' = net vertical abstraction.

Iterating Alternative Direction Implicit Explicit (IADIE) finite difference scheme has been applied for solving Eq. 3 and Eq. 1 to generate head field and corresponding velocities and concentration fields. This simulation model is linked externally with the optimizer, to arrive at closest match between simulated and observed concentration distribution.

Optimization problem formulation

The objective of the optimization problem is

$$\text{Minimize } Z = \sum_{i\in I}\left(C_i^{obs} - C_i^{simu}\right)^2 \qquad (4)$$

such that $C = f(X, Y, W)$

subject to

$$W_j \geq 0 \quad j=1, 2\ldots., n; \; X_L \leq X \leq X_U \; ; \; Y_L \leq Y \leq Y_U \qquad (5)$$

where C_i^{obs} = observed concentration at node i , C_i^{simu} = simulated concentration at node i, W_j = point source flux, $i \in I$ where I = set of nodes at which observed concentration data are available, X (={x_1,x_2…,x_n}) = x coordinate vector of point sources, Y (={y_1,y_2,….,y_n}) = y coordinate vector of point sources, n = number of unknown sources and C = simulated concentration vector which is a function of the unknown sources location and fluxes. Thus Decision variables are X, Y and W. n is also a decision variable but it is not used as an explicit variable. Exhaustive Search technique was employed to solve the above posed optimization problem.

3. Model Illustration

The model developed has been illustrated by a hypothetical two dimensional study area, shown in Fig. 1. Observed concentration field was needed for demonstrating the model applicability. It was generated by simulation model for assumed source flux values and known source location. This generated concentration field was then used as an input to the linked simulation optimization model, masking the assumed source flux values and known source location.

3.1. Study Area and Database

Study area of dimension 549 m×732 m was taken and is shown in Fig. 1. The north and south boundaries were considered as impermeable flow and no transport boundaries while east and west boundaries were taken as constant head and concentration boundaries. Two pollution sources (S1 and S2) were there in the study area, the location of which is shown in the Fig. 2. A pond was located in the area, which was considered free from contamination. The flow and transport parameters used in the simulation model are given in Table 1.

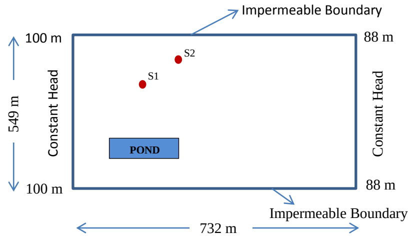

Figure 1. Study Area

Table 1. Simulation model parameters

Parameters	Value
T_{xx} and T_{yy} (m^2/d)	26.35
Grid spacing in x and y direction, Δx , Δy (m)	91.5
Longitudinal dispersivity, α_L (m)	40.0
Transverse dispersivity,α_T (m)	9.6
Aquifer Thickness, b (m)	30.5
Effective porosity, ϕ	0.2
Pond Recharge (m/d)	0.011
Source flux (S1 and S2) (kg/m^2/d)	31.7

3.2 Observed Concentration field generation

The study area was divided into grids of size 91.5×91.5 m each, shown in Fig. 2. Initial concentration of pollutant is assumed to be zero in the groundwater. Pollution sources were assumed to release conservative pollutant at a uniform rate throughout the activity period. The corresponding steady state concentration field was generated by solving the solute-transport equation numerically, employing the parameters and the assumed source flux listed above. Locations of the sources are given in Table 2.

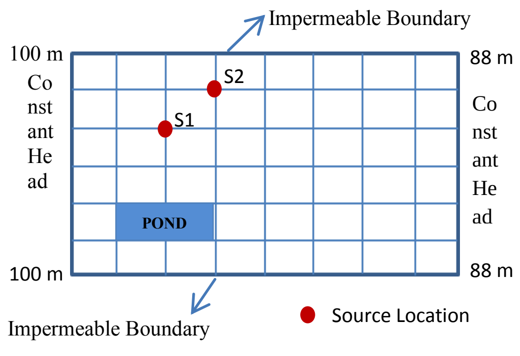

Figure 2. Finite Difference Grid for the study area

Table 2 Source Locations

Source	S1	S2
X (m)	274.5	183
Y(m)	549	457.5

3.3 Model Runs

The model was run by assuming a particular number of source (n let) and the decision variables varying accordingly (3n). For n=1, the limits for x and y are given below

$91.5 \leq x \leq 640.5$

$91.5 \leq y \leq 457.5$

i.e. the entire study domain was searched.

For n=2, the boundary constraints for the location coordinates were

$200 \leq x\_1 \leq 350$

$500 \leq y\_1 \leq 600$

$150 \leq x\_2 \leq 250$

$400 \leq y\_2 \leq 500$

4. Results

Results obtained for different number of sources is given in Table 3. For n=1, the source location and flux identified did not reproduce a better match between the observed and simulated concentration field. Hence the objective function value was high i.e. 74.1. For n=2, the objective function value did reduced to 0.0911, representing a close enough match between observed and simulated concentration filed. Thus the value chosen for n was 2 and corresponding optimal source location and flux chosen as the solution to the source identification problem.

Table 3 Identified results for different number of pollution sources

Actual source location (m)	Actual source flux (kg/m2/d)	No. of Sources	Identified Location (m)	Identified source flux (kg/m2/d)	Objective Function
(274.5,549.5) (183,457.5)	31.7 31.7	n=1	(138, 412)	36.0	74.01
		n=2	(260.8,554.4)	31.47	0.0911
			(140.7,453.1)	31.47	

5. Conclusion

From the results it is evident that the model is generally able to identify the source characteristics, i.e. the location of the pollutant sources and source flux. There was some deviation in the second source flux location from the actual source location, which could be because of the numerical errors or due to inadequate convergence during optimization.

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