

GROUNDWATER POLLUTION SOURCE IDENTIFICATION FROM LIMITED MONITORING WELL DATA

PART 1 — THEORY AND FEASIBILITY

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Summary

This paper describes a numerical technique for identifying and locating a specific groundwater pollution source using data from a small number of monitoring wells. The technique, a modified finite element model, uses a unique system sensitivity theorem and is iterative in that a series of estimates and verifications are made until convergence occurs at the actual source.

After description of the technique, a hypothetical problem is solved illustrating the computational procedure. A continuation of the study will illustrate the technique, using actual data from monitoring wells and known pollution sources.

Introduction

Having sufficient observation well data on a particular pollutant in the groundwater, one can plot concentration contours which will hopefully identify the pollution source [1]. However, even with a large amount of data, results are approximate at best. Furthermore, the time involved in collecting and analyzing the samples is large and the subsequent cost can be prohibitive.

A far more practical, and in many cases equally accurate, procedure is to use a computer model to simulate the flow with a limited amount of well data to upgrade the solution as it is in progress. In general, these models assume constant dispersivity of a contaminant in the aquifer and a steady state flow field, which are reasonable first approximations. In this manner, locating the pollution source is now equivalent to solving the identification problem of a linear dynamic system.

The aquifer parameter identification problems, or so called inverse problems, have been investigated for the past 10–15 years. Faust and Mercer [2] give a brief account of its recent development. In general, the calculation procedure for groundwater flow consists of finding a set of parameters (transmissivity, storage coefficient, sources, etc.) that minimizes deviations between observed and calculated values of hydraulic head. Thus, for steady state flow

problems, the criterion adopted to define the optimal set of parameters is to minimize:

$$\sum_{i=1}^m (h_i - \tilde{h}_i)^2 \quad (1)$$

where h_i and \tilde{h}_i are the observed and calculated heads at node i for a total of m observations. For the unsteady state flow problems the criterion function is the minimization of:

$$\sum_{i=1}^m \sum_{j=1}^T (h_{i,j} - \tilde{h}_{i,j})^2 \quad (2)$$

where $\tilde{h}_{i,j}$ and $h_{i,j}$ are the calculated and the observed heads made at the i th discretized point at time t_j , where $j = 1, 2, \dots, T$.

Several methods are available in order to achieve the minimization. Cooley [3] derived the modified Gauss—Newton procedures after linearizing the steady state equation using a similar technique to that used by Yeh and Taux [4]. Frind and Pinder [5] solved the inverse problem for transmissivity by the Galerkin finite element approach using steady state hydraulic heads as input data. For the dynamic system, Yeh [6] presents a good review on the methods of aquifer parameter estimation for unsteady state flow in an unconfined aquifer. Methods such as quasi-linearization, maximum principle and gradient method, influence coefficient methods and the minimax-linear programming approach have been presented in detail for achieving the minimization.

The application of the system's approach, however, for the identification of a groundwater pollution source similar to that for aquifer parameter identification seems to have been overlooked by previous researchers. Only recently a method based on the combined use of linear programming and simulation has been proposed [7]. In fact, if a steady-state flow field is assumed, the system control equation is linear. The criterion is then the minimization of the following expression:

$$J_t = \sum_{j=1}^m (u_{i,t} - \tilde{u}_{i,t})^2 \quad (3)$$

in which $\tilde{u}_{i,t}$ and $u_{i,t}$ are the calculated and observed concentration for the i th well, corresponding to time t . The matrix equation resulting from the finite element discretization for the mass transport equation can be written:

$$M\{\dot{c}\} + (K - A + E)\{c\} = \{p\}. \quad (4)$$

The notations are defined later in eqns. (10)—(15). The location and the strength of the pollution source are contained in the vector $\{p\}$. The estimate, $\{\tilde{p}\}$, approaches the true value of $\{p\}$ as J_t approaches a minimum

value. The method adopted in this study for achieving the minimization is based on system sensitivity theory.

The system sensitivity theory is a branch of modern control theory. Control engineers often face the assignment to design highly sophisticated dynamic systems with prescribed or optimal behavior on the basis of a mathematical model. The results are then useless in practice if they prove to be very sensitive to parameter changes. With the use of feedback, the sensitivity analysis provides the engineers with methods for investigating or minimizing the effects of such parameter deviation. The theory for sensitivity analyses is known as sensitivity theory.

One of the applications of the sensitivity theory is for parameter identification. Equation (4) represents the system equation of groundwater pollution transport with state variable $\{c\}$, and $\{p\}$ is the parameter to be identified. With the feedback (c as measured), $\{\tilde{p}\}$ is improved at each subsequent time by calculating the so called trajectory function, $\{\partial J/\partial p\}$, and adding it to $\{\tilde{p}\}$ for the next time step. Some mathematical details will be described in the next section.

This paper, which follows one showing the essential outline of the technique [8], is aimed at illustrating feasibility using hypothetical data. There is sufficient information presented here, however, that one needs not refer back to the original reference. This paper will be followed by a paper which uses actual field data. The following stage is to extend the technique to the solution of three-dimensional problems. This information will be forthcoming as the program continues.

Theoretical background

Governing equations of pollution transport

The governing equation of pollutant transport in porous media is the following (Freeze and Cherry [9]):

$$nR \frac{\partial c}{\partial t} = n \left[\frac{\partial}{\partial x} \left(D_{xx} \frac{\partial c}{\partial x} + D_{xy} \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial y} \left(D_{yx} \frac{\partial c}{\partial x} + D_{yy} \frac{\partial c}{\partial y} \right) \right] - \left[\frac{\partial}{\partial x} (V_x c) + \frac{\partial}{\partial y} (V_y c) \right] - n\lambda R c + Qc^* \quad (5)$$

in which c = concentration of the pollutant; $R = 1 + \rho_s k/n$ = retardation factor; ρ_s = bulk density of the porous medium; k = distribution coefficient of the pollutant; n = porosity of the porous medium; D_{xx} , D_{xy} , D_{yx} , D_{yy} = component of dispersion tensor; V_x , V_y = Darcian velocity component; λ = 1st order decay constant; c^* = concentration of the source fluid; and Q = flow rate of the source fluid.

Let L denote the operator on c in eqn. (5), thus

$$Lc = 0 \quad (6)$$

For the finite element method:

$$c \sim \hat{c} = \Sigma c_i(t)N_i = \{N\}^T \{c\} \quad (7)$$

where $\{N\}^T$ is the transpose of the interpolation function, $\{N\}$. The residue becomes $L\hat{c}$. The principle of Galerkin method requires that

$$\langle L\hat{c}, W_i \rangle_B = 0. \quad (8)$$

Equation (8) states that the inner product of $L\hat{c}$ and the weighting function W_i over the solution domain B vanishes.

The integrations in eqn. (8) are now carried out and the results are expressed in matrix and vector notation as follows (Yeh and Ward [10])

$$\{c\}^T [M\{\dot{c}\} + (K - A + E)\{c\} - \{p\}] = 0 \quad (9)$$

in which

$$\{\dot{c}\} = \left\{ \frac{dc}{dt} \right\} \quad (10)$$

$$K = \iint_B \left[nD_{xx} \left\{ \frac{\partial W}{\partial x} \right\} \left\{ \frac{\partial N}{\partial x} \right\}^T + nD_{xy} \left\{ \frac{\partial W}{\partial x} \right\} \left\{ \frac{\partial N}{\partial y} \right\}^T + nD_{yx} \left\{ \frac{\partial W}{\partial y} \right\} \left\{ \frac{\partial N}{\partial x} \right\}^T + nD_{yy} \left\{ \frac{\partial W}{\partial y} \right\} \left\{ \frac{\partial N}{\partial y} \right\}^T \right] dx dy \quad (11)$$

$$A = \iint_B V_x \left\{ \frac{\partial W}{\partial x} \right\} \{N\}^T + V_y \left\{ \frac{\partial W}{\partial y} \right\} \{N\}^T dx dy \quad (12)$$

$$E = \iint_B n\lambda R \{W\} \{N\}^T dx dy \quad (13)$$

$$M = \iint_B nR \{W\} \{N\}^T dx dy \quad (14)$$

$$\{p\} = \iint_B Qc^* \{N\} dx dy + \oint_S \left[\left(nD_{xx} \frac{\partial c}{\partial x} + nD_{xy} \frac{\partial c}{\partial y} - V_x c \right) n_x + \left(nD_{yx} \frac{\partial c}{\partial x} + nD_{yy} \frac{\partial c}{\partial y} - V_y c \right) n_y \right] \{W\} ds. \quad (15)$$

The area integral on the right hand side of eqn. (15) represents the "load" from the "source fluid", while the line integral accounts for the boundary contribution. If the boundary conditions prescribed are of Neumann type with normal derivatives equal to zero, the line integral on the right hand side of eqn. (15) disappears and

$$\{p\} = \iint_B Qc^* \{N\} dx dy. \quad (16)$$

For a single isolated source Qc^* can be expressed as

$$Qc^* = q\delta(x - x^*, y - y^*) \quad (17)$$

where δ is the Dirac Delta function, (x^*, y^*) are the global coordinates of the source point location and q is the strength of the source. Now, substitute eqn. (17) into eqn. (16) and integrate. It can be shown that

$$\{p\} = \begin{pmatrix} 0 \\ 0 \\ \dot{q} \\ \vdots \\ 0 \end{pmatrix} \quad (18)$$

The vector has zero entries except at the "source" node where the entry value is q .

Two most important advantages of the finite element method over the finite difference method are its ability to handle complex boundaries and normal derivatives. In the time dimension, these advantages are not present so the finite difference method will be used for the time derivative in eqn. (9).

With finite difference in time, eqn. (9) becomes

$$\left[\frac{M}{\Delta t} + \mu(K - A + E) \right] \{c\}_{t+\Delta t} = \left[\frac{M}{\Delta t} - (1 - \mu)(K - A + E) \right] \{c\}_t + [\mu\{p\}_{t+\Delta t} + (1 - \mu)\{p\}_t] \quad (19)$$

in which $\mu = 1$ for backward-differences and $\mu = 0.5$ for the Crank—Nicolson differencing scheme.

The problem of locating a pollution source from limited well data is to identify the source vector $\{p\}$ in eqn. (9) or (19) for some given entry values in the concentration vector $\{c\}$ at some discrete instant in time. The method to be introduced for the identification is the method of system sensitivity.

Method of system sensitivity

Let $\{u\}_t$ be the measurement vector of concentration from m observation wells at time t , then

$$\{u\}_t = F\{c\}_t \quad (20)$$

where F is the location matrix of the observation wells. If $\{\tilde{u}\}_t$ represents the estimate of $\{u\}_t$ using an estimated $\{p\}$ in eqn. (9), i.e.,

$$M\{\tilde{c}\} + (K - A + E)\{\tilde{c}\} = \{\tilde{p}\} \quad (21)$$

and

$$\{\tilde{u}\} = F\{\tilde{c}\}, \quad (22)$$

the error between the estimates and the measurements at time t is

$$J_t = \{u - \tilde{u}\}_t^T \{u - \tilde{u}\}_t. \quad (23)$$

The system sensitivity theorem [11] provides a recurrence formula for $\{\tilde{p}\}$, (estimate of $\{p\}$), for the next time step in a manner so as to minimize J_t . When J_t approaches a minimum value, $\{\tilde{p}\}$ approaches to real $\{p\}$.

$$\{\tilde{p}\}_{t+\Delta t} = \{\tilde{p}\}_t - \Delta \left\{ \frac{\partial J}{\partial p} \right\}_t \tag{24}$$

in which Δ is the step size, ranging between 0 and 1 for normalized elements.

Differentiating eqn. (23) with respect to $\{p\}$ leads to

$$\left\{ \frac{\partial J}{\partial p} \right\}_t = 2\{u - \tilde{u}\}_t^T F \left[\frac{\partial c}{\partial p} \right]_t \tag{25}$$

The matrix $[\partial c/\partial p]$ can be obtained from eqn. (9) as follows. Differentiate eqn. (9) with respect to $\{p\}$, then

$$M \left[\frac{\partial \dot{c}}{\partial p} \right] + (K - A + E) \left[\frac{\partial c}{\partial p} \right] - I = 0, \tag{26}$$

where I is an identity matrix. Using the finite difference scheme for the time derivative, eqn. (26) becomes

$$\left[\frac{M}{\Delta t} + \mu (K - A + E) \right] \left[\frac{\partial c}{\partial p} \right]_{t+\Delta t} = \left[\frac{M}{\Delta t} - (1 - \mu)(K - A + E) \right] \left[\frac{\partial c}{\partial p} \right]_t + I \tag{27}$$

Note that $[\partial c/\partial p]_{t+\Delta t}$ is a matrix and it is convenient to express eqn. (27) as a system of linear equations with unknowns $\{\partial c/\partial p_i\}_{t+\Delta t}$:

$$\left[\frac{M}{\Delta t} + \mu (K - A + E) \right] \left\{ \frac{\partial c}{\partial p_i} \right\}_{t+\Delta t} = \left[\frac{M}{\Delta t} - (1 - \mu)(K - A + E) \right] \left\{ \frac{\partial c}{\partial p_i} \right\}_t + \{I_i\}$$

$$i = 1, 2, \dots, n \tag{28}$$

in which

$$\{I_i\} = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \leftarrow \text{ith}$$

and n is the number of nodal points. The system equation can easily be solved because all $\{\partial c/\partial p_i\}_{t+\Delta t}$ have the same constant coefficient of $(M/\Delta t + K - A - E)$ which is needed to be triangularized only once.

Overview of the computational procedures and the computer program DREXEL

The flow diagram shown in Fig. 1 illustrates the dynamic iteration for the identification of $\{p\}$.

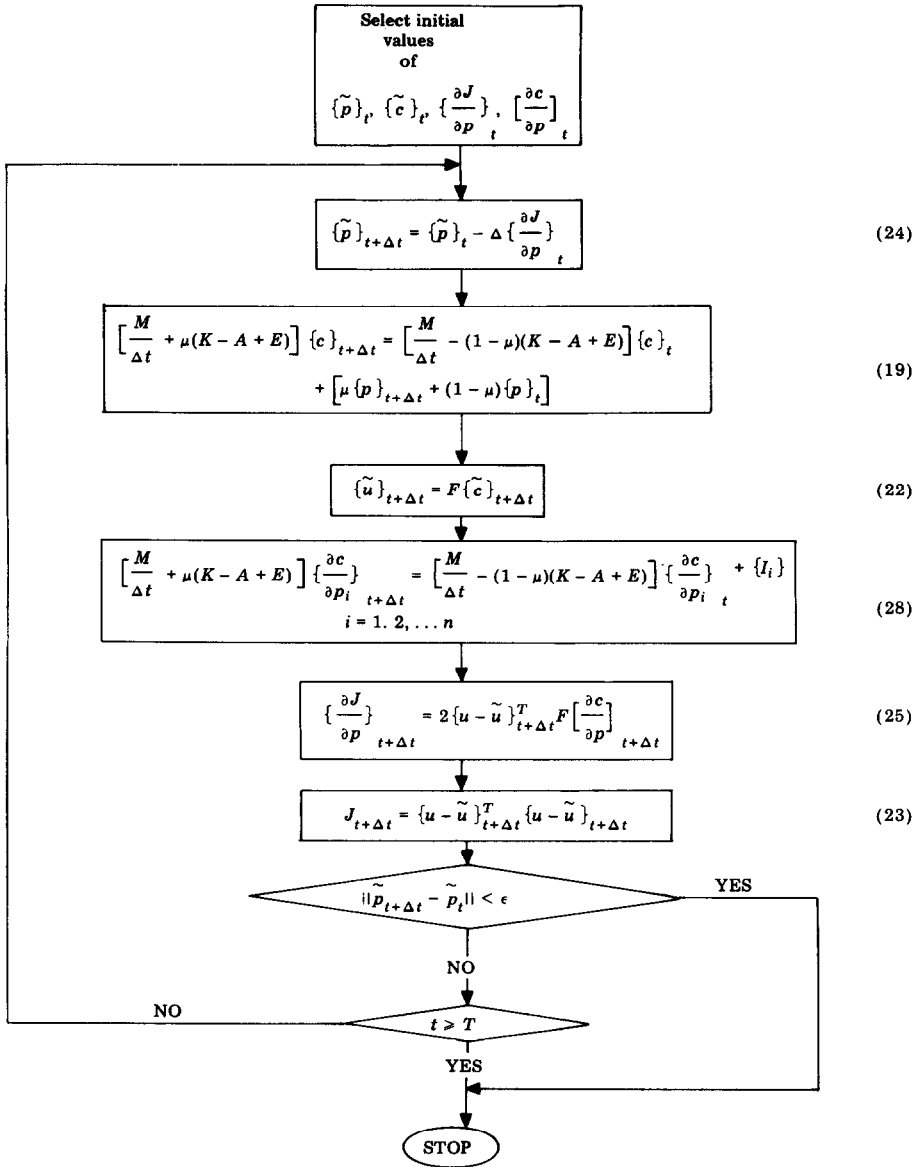


Fig. 1. Flow diagram showing iteration procedure for identification of {p}.

A computer program, DREXEL, has been developed based on the aforementioned algorithm. It is important that the groundwater pollution transport model incorporated in the computer program is numerically stable with-in reasonable accuracy.

In DREXEL three major options are implemented in order to achieve these goals, i.e.,

- conventional Galerkin scheme/upstream weighted scheme;
- mass lumping technique/no mass lumping;
- Crank—Nicolson scheme/backward time differencing.

When the convection terms in eqn. (5) are as important as the dispersion terms, it is sometimes advantageous to use asymmetric weighting functions different from the interpolation functions in the spatial discretization (Huyakorn and Nilkuha [12], Heinrich et al. [13]). Such an upstream weighted scheme has been shown to be adequate (Huyakorn and Pinder [14]). The problem of numerical oscillation associated with convectively dominated flow can then be overcome.

In general, a backward-difference formulation for time derivatives provides the best numerical stability. However, the Crank—Nicolson scheme yields better results. Gureghian et al. [15] reported that, in many cases, the lumped-mass matrix would result in a better solution, in particular if it is used in conjunction with the central- or backward-difference time marching. Under other circumstances, it is preferred to use the consistent mass matrix (mass matrix without lumping). Therefore, options of lumping/no lumping, and of different time differencing schemes are provided in the computer program.

Methodology and results for source identification

Unlike the conventional method of requiring numerous observation wells and samples, the methodology developed here is to analyze the available data at each time for each sequential well system using a numerical model called DREXEL. The outcome of the numerical model will indicate the favorable direction and/or location of additional well(s) for the next step. An operative method of such kind will substantially reduce the costs of not only the number of required observation wells but also of the required number of samples at each specific well.

For the development and the testing of the methodology using DREXEL, the error in the field data supplied to the computer runs must be known, or kept to a minimum, so that the testing results solely reflect the characteristics and the capabilities of the model. The tests were done by applying DREXEL to a site where the concentration of a pollutant species at observation wells was computer-generated, simulating a set of ideal field measurements.

The methodology consists of several steps. They will be outlined first and then illustrated through an example.

The procedure of the method is as follows:

- (1) Discretization of the site.
- (2) Computing the groundwater velocity field.
- (3) Organizing the concentration data sampled at the existing wells and execution of the first computer run of DREXEL.

- (4) Analyzing the source distribution vector $\{p\}$ and proposing the next additional well(s) based on the analyses.
- (5) Preparation of the new concentration data set and execution of the subsequent computer run of DREXEL.
- (6) Repeating steps (4) and (5) until $\{p\}$ does not vary compared with the previous computer run. The source location is then shown by $\{p\}$.
- (7) Determination of the source strength.

As an example, consider that a certain constituent of groundwater pollutant has been detected at three observation wells in a rectangular site (1800 ft \times 900 ft). The concentrations and the sampling time are shown in Table 1. For simplicity, the seepage velocity field through the aquifer is assumed steady and uniform with $V_x = 40$ ft/day, $V_y = 1$ ft/day and the dispersion coefficients are $D_{xx} = 80$ ft²/day and $D_{yy} = 10$ ft²/day. A source is emitting the pollutant at a constant rate from an unknown location within the site. We want to identify the pollution source using the methodology just described.

TABLE 1

Normalized concentration data

Well no.	Conc. at time = t_1	Conc. at time = $t_1 + 51$ days
23	9.16×10^{-7}	2.19×10^{-6}
73	3.25×10^{-6}	4.83×10^{-5}
78	1.15×10^{-5}	1.35×10^{-3}

Step 1. The site is discretized into 81 rectangular elements of equal size. The numbering system of the grid is shown in Fig. 2.

Step 2. The velocity field is steady and uniform; $V_x = 4$ ft/day and $V_y = 1$ ft/day for all the nodes.

Step 3. The time of origin is adjusted until the concentration measurements are best fitted to straight lines against time for each observation well. For this example problem, the time span between the first observations and the estimated time of origin is 21 days. The concentration data are then organized and shown in Table 2. The input data file prepared accordingly is supplied to the computer for the execution of the first computer run of DREXEL. In the computation, the concentration at an observation well at any instant is approximated by linear interpolation between the two nearest consecutive measurements at that well.

Step 4. The first run of DREXEL yields the source distribution vector $\{p\}$.

At the end of 72 days the computed $\{p\}$ is obtained and is plotted as in Fig. 3. The positive entry of $\{p\}$ is the source while the negative is the sink.

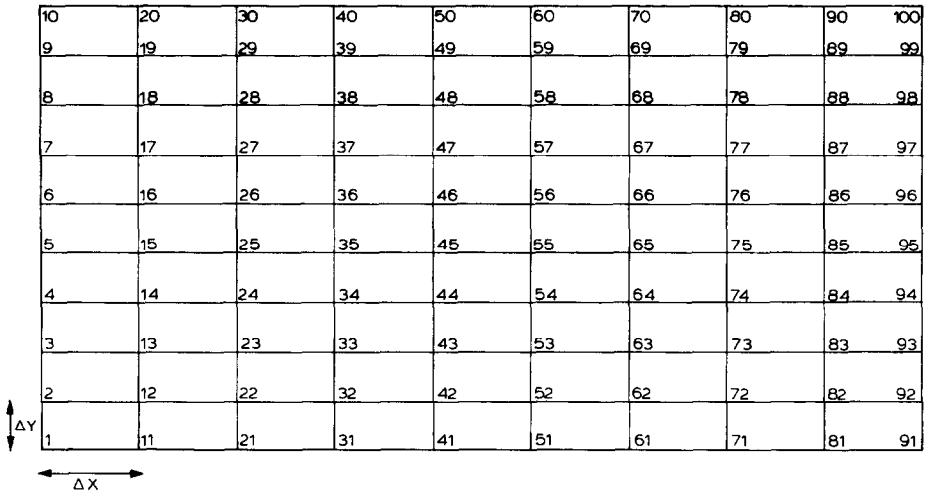


Fig. 2. The grid system.

TABLE 2

Input normalized concentration data for three wells

Well no.	Conc. at time = 0	Conc. at time = 21 days	Conc. at time = 72 days
23	0	9.16×10^{-7}	2.19×10^{-6}
73	0	3.25×10^{-6}	4.83×10^{-5}
78	0	1.15×10^{-5}	1.35×10^{-3}

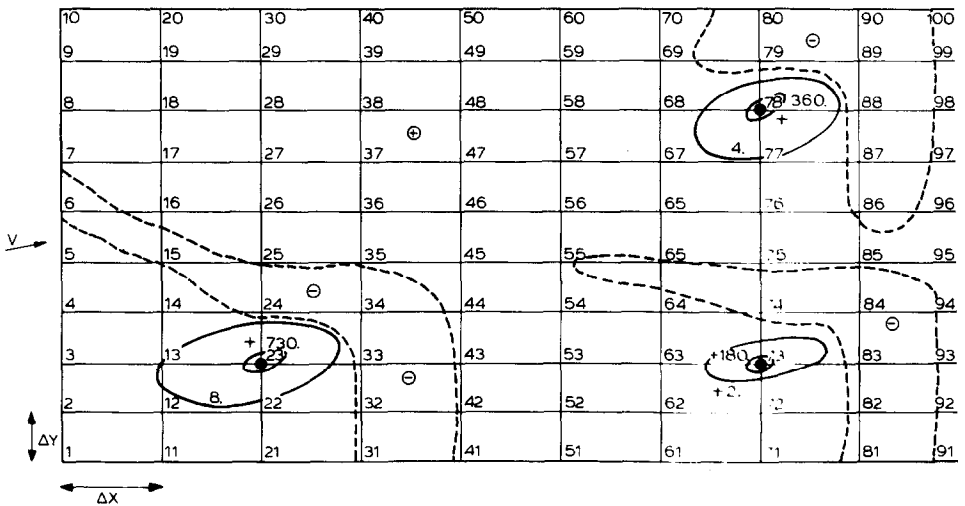


Fig. 3. Source distribution with three observation wells, nos. 23, 73 and 78.

The results represent the best combination of sources and sinks, which minimizes the sum of error squared between the estimated and the measured concentration at the three observation wells.

From Fig. 3 it can be seen that there are three primary sources with strength of about the same order of magnitude at nodes no. 23, 73 and 78. Among them the source at no. 23 is the strongest, suggesting that the search of pollution source location should begin in the neighborhood of node no. 23.

Next we want to determine the direction relative to node no. 23 for proposing additional well(s), and whether it will be downstream or upstream of node no. 23.

Should the real pollution source be upstream of no. 23, the concentration at no. 23 would be higher than that at no. 73 and at no. 78 for all time, because the latter are further downstream of the source. However, the concentration data in Table 2 records the opposite. It becomes obvious that we shall propose a well drilled at node no. 34 (downstream of no. 23) for additional groundwater sampling.

Step 5. A new set of concentration data including the new well at node no. 34 is then compiled as shown in Table 3. DREXEL computes $\{p\}$ at the end of 106 days. The results are obtained and plotted in Fig. 4.

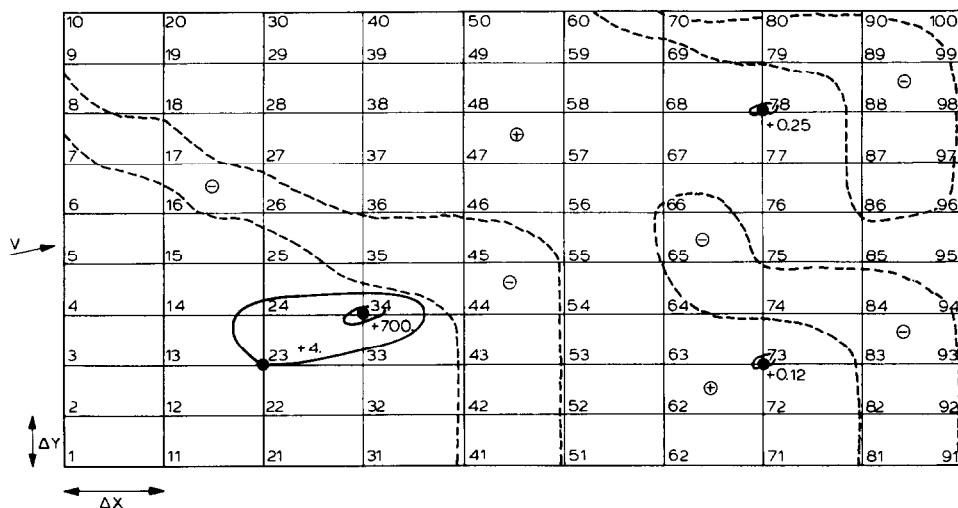


Fig. 4. Source distribution with four observation wells, nos. 23, 73, 78 and 34.

Step 6. The fact that the strongest source point shifts from no. 23 to no. 34 while the strength of the source at no. 23, 73 and 78 reduces indicates that the proposed new well (no. 34) has been located in the correct direction (closer to the pollution source). Thus, the second well is proposed to be downstream of no. 34 (at node no. 45).

Step 7. Another set of concentration data at the end of 128 days is prepared (Table 4) and $\{p\}$ is computed by DREXEL. It is presented in Fig. 5.

TABLE 3

Input normalized concentration data for four wells

Well no.	Conc. at time = 0	Conc. at time = 21 days	Conc. at time = 72 days	Conc. at time = 106 days
23	0	9.16×10^{-7}	2.19×10^{-6}	1.44×10^{-5}
73	0	3.25×10^{-6}	4.83×10^{-5}	2.79×10^{-5}
78	0	1.15×10^{-5}	1.15×10^{-5}	5.89×10^{-3}
34	0	—	—	1.08×10^{-2}

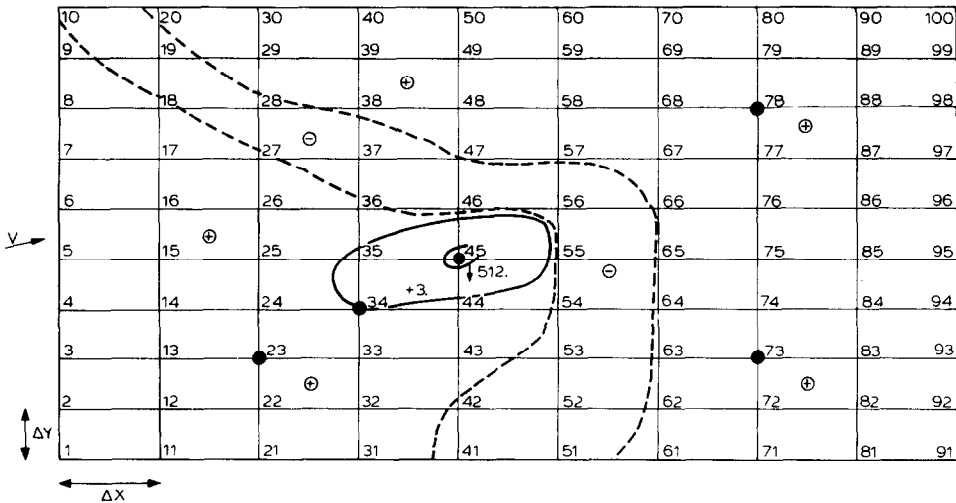


Fig. 5. Source distribution with five observation wells, nos. 23, 73, 78, 34 and 45.

Step 8. The strongest source point shifts further from no. 34 to no. 45 and the strength of the source at all other nodes drops drastically. This shows a very favorable sign of the source being located. One more well is then proposed downstream of no. 45, at node no. 56.

Steps 9 and 10. With the new data set (Table 5) DREXEL again computes the source vector $\{p\}$; it is shown in Fig. 6. This time the source point stays at no. 45 and the general pattern of the distribution is identical to the previous one. Thus, the source location is identified to be at node no. 45.

Step 11. The source strength is determined using the other version of the computer code DREXEL for computing pollution transport only. Since the source location has been identified, a numerical simulation can be performed using DREXEL to obtain the distribution of the concentration at any given time.

At node no. 45 a source strength (=572), obtained from step 10, is assigned for the initial simulation run. The simulated results at each well compare quite well with the observation values except that they are off by an almost

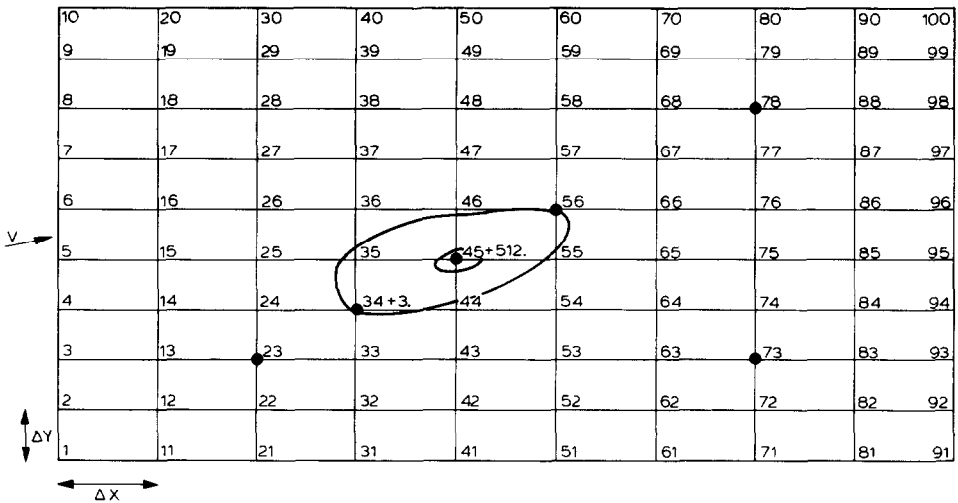


Fig. 6. Source distribution with six observation wells, nos. 23, 73, 78, 34, 45 and 56.

constant factor of about 2. Next, the source strength is adjusted (to 929), until the simulated and the measured concentrations at the observation wells are in good agreement.

Conclusions and recommendations

The general problem of locating a pollution source by having data from a limited number of observation wells is quite challenging, yet worthwhile, due to the shorter time and lower costs involved over the conventional method of pollutant contour mapping. The basic tool used for this purpose is the finite element method (FEM). While a good deal of information exists on this subject as far as taking a known source and mapping out its migration is concerned, the inverse problem of finding the source from a limited number of observation points is more difficult. This concept was used in this study.

A still more important point is that of the available methodologies, the application of a systems approach (as described herein) being a new solution technique. With a steady-state flow field assumed, the system control equation is linear and the criterion function can be minimized to an arbitrarily selected value.

The method of system sensitivity was described in the paper along with related theoretical considerations. The analytic formulation was the basic objective of an earlier paper [8] although parts were repeated here for the sake of clarity. This paper extended the work to the solution of a hypothetical problem. Its solution was seen to accurately identify a pollution source with a minimum number of iterations. Thus, armed with a computer code, DREXEL, actual field data will be used for Part 2 of this overall program.

Extension beyond this point will be the adaptation of the code to the

three dimensional problem: first, a test of feasibility with hypothetical data, then evaluation with real field data.

Hopefully, the completed program will identify pollution sources from data from a very small number of monitoring wells. The final program also holds the promise of being able to locate where additional wells should be located for an on-going pollution scheme.

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