AUTOMATIC CALIBRATION FOR SALT WATER INTRUSION PROBLEMS BY USING AN OPTIMISATION TECHNIQUE

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ABSTRACT

A new scheme for indirect calibration is developed. NAG subroutines, which are available in the computer library, are coupled with SWICHA for investigating flow and salt transport parameters. The SWICHA model is a three dimensional finite element model. It can be used easily in salt water intrusion problems, or groundwater resource evaluation. A computer programme has been created to accelerate the calibration process. The application of the optimisation technique using such developed programme is applied to both hypothetical and real data.

Keywords: Environmental Aspects Of Salt Water Intrusion- Pollution Of Ground Water -Numerical Modelling-Automatic Calibration.

INTRODUCTION

Calibration of a model means the selection of model parameters such as permeability, dispersivity, leakage etc. to give the best output of variables e.g. potential head and salt concentration values in comparison with field data. Generally, there are two approaches for automatic calibration, the direct approach and the indirect approach.

In the direct approach, the unknown model parameters are treated as dependent variables in the governing equations and the output variables are treated as independent or known variables. This means that target values for the output known variables must be the input for all nodes in a numerical model grid. These target values are known only at points where there are field observations, making it necessary to estimate the values elsewhere in the grid. Assigning parameter values to the grid is difficult because the model requires values for each node, cell, or element and field data are typically sparse. Interpolation of measured data points can help in defining the spatial variability over the problem domain, or parameter values may be assigned to the rest of the nodes using hydrogeological judgement. Direct solutions are prone to instability [1]. Furthermore, they do not recognise measurement errors.

The indirect approach is similar to performing trial and error calibrations. The problem is solved repeatedly for different values of the model parameters until a good fit between the field data and the computed values of potential and salinity is obtained. However, a code can be devised which automatically checks the progress of the solution and adjusts the model parameters in a systematic way in order to minimise the objective function as quickly as possible [1].

With the invention of high speed digital computers, mathematical optimisation has become a widely used technique for scientific and engineering problems. The theory and practice of optimisation

has been developed rapidly and found increasing application in various fields, such as statistics, aerodynamics, engineering, operational research and many more. Nowadays, optimisation techniques are well established and documented in many standard referenceson automatic calibration [2]. The main objective of any optimisation problem is to minimise or maximise a scalar quantity given by an objective function such as:

$$E = f(X) \tag{1}$$

in which E is the scalar quantity, and f(x) is the objective function. x is a vector which may have one or more variables. These variables may be the model parameters to be identified or may be dependent upon these parameters.

The problem at hand, like many other engineering problems, requires minimising a function consisting of functions of one or more independent variables and not directly the system parameters. The objective function then takes a series of values at specific sample points of the independent variables. So the objective function in this case is made up of errors, e_j, at the individual sample points, i.e.

$$E=f(e_j) \tag{2}$$

where j = 1, 2,..... m.

m is the number of sample points selected. The basic problem now is to minimise E as in any other optimisation process. To apply standard methods of optimisation, the problem needs to be restated so that the individual errors comprising E are combined into one scalar quantity usually one of two criteria, the Minimax Error Criterion or the Least Squares Error Criterion[2]. The later is going to be used through out this research.

Least Squares Error Criterion [2]

In fact, the maximum error may occur at any point in the studied domain and perhaps at different points in depth. This tends to make the optimisation process jumps here and there and so becomes relatively complex. The additive errors over the whole domain are not directly constrained.

The objective function, according to the Least Squares Error Criterion is given as the minimum value of:

$$E=\sum_{j=1}^{m} [w_j e_j]^2 \tag{3}$$

By dropping the weighting factor w_j, i.e. giving equal importance to all error values, the objective function can be written as:

$$E=\sum_{j=1}^{m} [e_j]^2 \tag{4}$$

For salt water intrusion, with a fully mixed zone approach, different forms of objective functions may be written for instance as:

$$E = \sum_{j=1}^{m} (\phi_o(j) - \phi_c(j))^2 \tag{5}$$

$$E = \sum_{j=1}^{m} (c_o(j) - c_c(j))^2 \tag{6}$$

$$E = \sum_{j=1}^{m} [\phi_o(j) - \phi_c(j)]^2 + \sum_{j=1}^{m} (c_o(j) - c_c(j)^2) \tag{7}$$

where m is the number of the samples, ϕ is the potential head, c is the salt concentration and o, c are subscripts denoting the observed and calculated values. The number of samples is taken to be the number of nodes of the grid.

Suppose a set of model parameters x_i results in a value for $E = E(x_i)$. We require a new set $x_i + Dx_i$ which will result in a reduction of E. Differentiating equation (4) partially with respect to each of the system parameters in turn gives

$$\frac{\partial E}{\partial x_i} = \sum_{j=1}^{m} 2 e_j \frac{\partial e_j}{\partial x_i} \tag{8}$$

where i = 1, 2.... n are the number of the system parameters. The complete set of partial derivatives can be represented in matrix form as

$$\begin{bmatrix} \frac{\partial E}{\partial x_1} \\ 0 \\ 0 \\ \frac{\partial E}{\partial x_n} \end{bmatrix} = 2 \begin{bmatrix} \frac{\partial e_1}{\partial x_1} & \cdots & \frac{\partial e_m}{\partial x_1} \\ \cdot & & \\ \cdot & & \\ \frac{\partial e_1}{\partial x_n} & \cdots & \frac{\partial e_m}{\partial x_n} \end{bmatrix} \begin{bmatrix} e_1 \\ \cdot \\ \cdot \\ e_m \end{bmatrix} \quad (9)$$

The left hand side of this equation is the Jacobian vector J of the objective function. In matrix form this can be stated as

$$J = 2 A F \quad (10)$$

where

$$A = \begin{bmatrix} \frac{\partial e_1}{\partial x_1} & \cdots & \frac{\partial e_m}{\partial x_1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \frac{\partial e_1}{\partial x_n} & \cdots & \frac{\partial e_m}{\partial x_n} \end{bmatrix} \quad (11)$$

and $F^T = [e_1\ e_2 \ldots e_m]$ (12)

Assuming that the objective function has continuous second partial derivatives, a second differentiation of equation 8, gives

$$\frac{\partial E}{\partial x_i \partial x_k} = 2 \sum_{j=1}^{m} \frac{\partial e_j}{\partial x_k} \frac{\partial e_j}{\partial x_i} + 2 \sum_{j=1}^{m} e_j \frac{\partial^2 e_j}{\partial x_i \partial x_k} \quad (13)$$

where k = 1, 2,....n the number of parameters. The usual least squares procedure assumes that the second term can be neglected. Hence, recognising () as the Hessian matrix, H [3], this equation becomes

$$H \approx 2 A A^T \quad (14)$$

The Jacobian vector and Hessian matrix of equations 10 and 14 can now be substituted in a simplified form of the equation of the Taylor expansion in matrix form as follows:

$$E(x+\Delta x) = E(x) + J \Delta x + H \Delta x^2 + \quad (15)$$

The increment Dx that is required is the array of Dx_i which minimises the change in E and is given by

$$\Delta x = - J/H \quad (16)$$

$$\Delta x = - [A A^T]^{-1} A F \quad (17)$$

The resulting process is often termed as the Gauss-Newton method. In general $A A^T$ has to be positive definite for this proto converge.

DESCRIPTION OF THE TECHNIQUE DEVELOPED FOR AUTOMATIC CALIBRATION

The use of an optimisation technique in the calibration of numerical models is considered to be an indirect approach. The chosen parameters in the calibration include flow parameters and salt transport parameters. This approach is similar to performing trial and error calibration in that the forward problem is solved repeatedly, the purpose of which is to minimise the discrepancy between the calculated and observed values of the potential and salt concentration.

The main steps of the new developed scheme are shown in flow chart of Figure (1). They can be summarised as follows:

1- Reading the input records: The input data includes: The initial guess of the parameters. These parameters are the saturated hydraulic conductivity in the three directions Kx, K_y and K_z, the longitudinal dispersivity a_L and the transverse dispersivity a_T. The leakage coefficient can be included with the above parameters if required. The real observed values of the potential and salt concentration are also included in this file. The numerical grid with the nodal coordinates and boundary conditions.

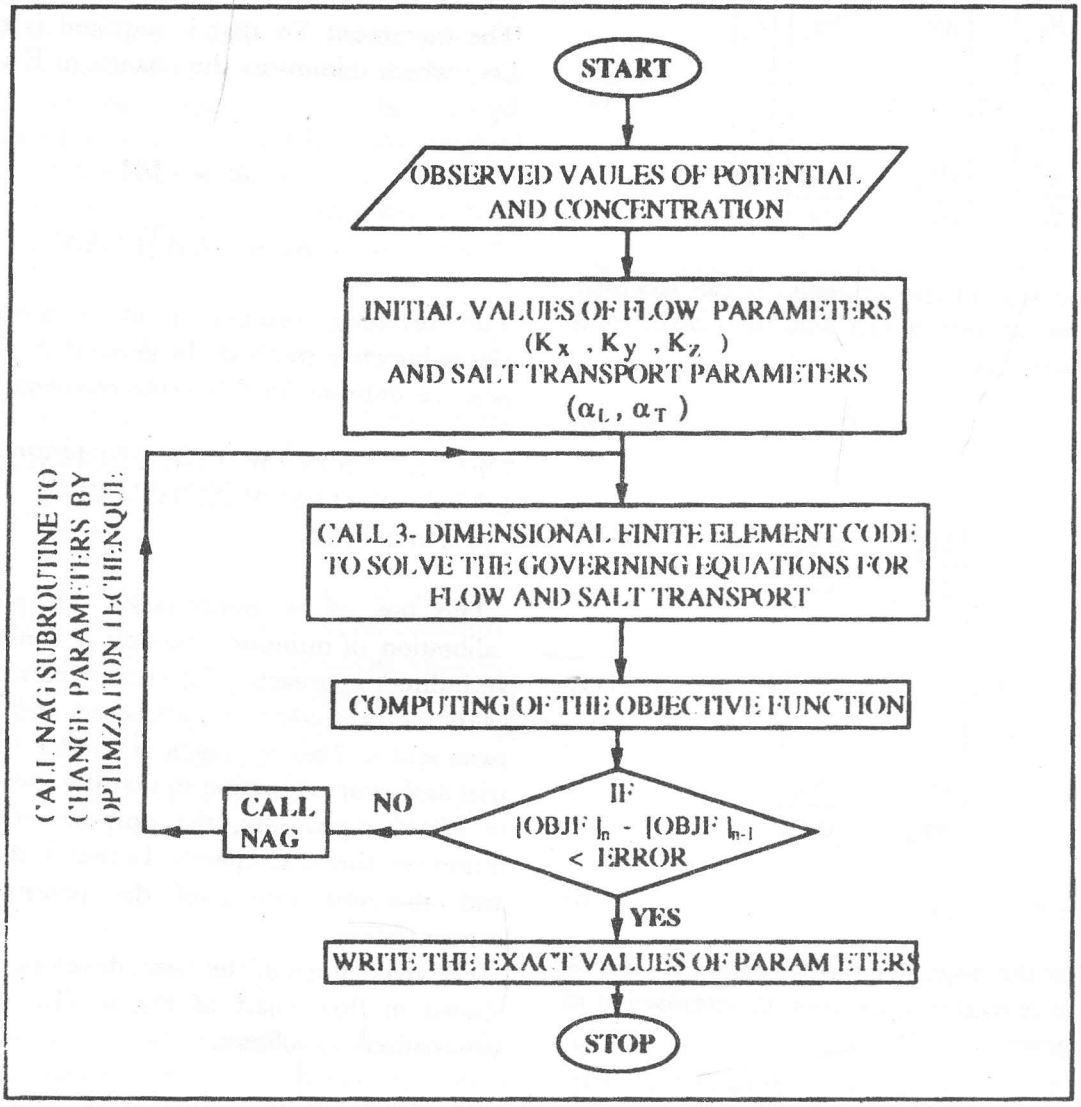

Figure 1. *Automatic Calibration procedures.*

2- **Calling the three dimensional programme (SWICHA):** SWICHA is considered in this scheme to be a subroutine. This subroutine is used to calculate the potential and salt concentration at every node of the domain. These calculations depend on the initial guesses for the different parameters. The details of the programme SWICHA were explained by Lester [4].

3- **Computing the objective function:** This is done by choosing one of the formulas prescribed in equations 5 to 7.

4- **Calling optimisation subroutine:** This is done by calling the NAG library [3]. This subroutine depends on the Least Square technique which is in turns based on the Gauss Newton method. There is no need to provide derivatives of the objective function in this technique. The subroutine itself calculates the derivatives numerically. The decisions about the values of the parameters for the next iteration, if required, are based on these numerical values of the derivatives.

5- **Repeating steps 2,3 and 4:** This procedure of calculations is repeated until the objective function does not change significantly between

two successive iterations.

Generally, there are three criteria that may be set for the termination of the optimisation process :

a- The number of maximum iterations may be fixed;

b- The maximum allowable change in the objective function may be provided;

c- The relative change in the objective function between two successive iterations is lower than certain accuracy. This criteria is adopted because the optimisation has to continue as far as it could go practically and this is suitable for automatic calibration.

The output of this code includes the values of the parameters for every iteration and the values of the associated objective functions.

APPLICATION OF THE TECHNIQUE

The developed model is applied to two different problems:

a- Problem with hypothetical data for which the solution is known.

b- Real problem: Biscayne aquifer in the Culter area near Miami.

HYPOTHETICAL PROBLEM

In this section the automatic calibration is achieved by using an optimisation technique which is applied to a known solution. A problem of salt water intrusion (Salt water upconing beneath a gallery) is solved and the simulated values of the variables (f(x,y,z), c(x,y,z)) are considered to be the observed data.

This hypothetical problem concerns the upconing of salt water beneath a collector well (gallery) pumping at a constant rate in the fresh water zone of a confined aquifer. The geometry of the problem, the boundary conditions and the true values of the parameters are depicted in Figure (2). A transient simulation is performed using a two -slices rectangular grid to represent the right half of the region as shown in Figure (2). The grid consists of 400 elements and 882 nodes. The nodal spacing in the x, y and z directions are uniform and equal to 5m, 2m and 50 m, respectively. As stated earlier the results of such solution are assumed to be the observed data. Then the values of the saturated hydraulic conductivities Kx, K_y, the longitudinal dispersivity, a_L, and the transverse dispersivity, a_T, are changed and an optimisation technique based on the gradient method [5] is applied to identify the true values for the parameters.

Four parameters, namely, the two ground water flow parameters (K_x, K_y)and the salt transport parameters (a_L, a_T) are optimised using the objective function of equation (7). Parameters whose values differ by significant percentage from their real values are used as the initial guess. The results are shown in Table (1).

From Tables (1-A), (1-B), and (1-C), it is observed that in the optimisation process a very small value is added to each parameter in turn and its effect on the objective function is observed. The Jacobian matrix elements are determined numerically. The decision on the direction and the amount of change of the parameters is taken at the 6 th and the 11th iteration Table (1-A). The number of iterations needed to minimize the objective function depends on the initial guess. In Table (1-A), the objective function changes from 1.64 to 0.43 at the sixth step, after little change occurred in the parameters in the first five iterations. This sudden change in the objective function is due to changes in all of the four parameters simultaneously. This was expected on the basis of the sensitivity analysis which showed how sensitive the objective function is when all parameters are changed at the same time. Comparing the first step in Tables (1-A), (1-B) and (1-C), the value of the objective function increases or decreases depending on the vertical anisotropy (K_x/K_y), regardless of the values of the permeability itself. The change of flow parameters has a more significant effect on the value of the objective function than the salt transport parameters. This is because the salt transport depends on the flow parameters implicitly. Although, there is no significant change in the value of objective function after iteration number 244 Table (1-C), the optimisation does not terminate because the relative change in the objective function is higher than the provided accuracy.

Generally, it is clear that the solution is stable and straight forward but a good initial guess of the parameters, which depends on field tests, will be very helpful in saving CPU time.

Case A : An Initial Guess Of Parameter's Values Deviating By Less Than 100% From Their Real Values.					
Iteration No.	Obj. Funct.	K_x[m/day]	K_y[m/day]	α_L[m]	α_T[m]
1	1.63857338	100.00	15.00	100.00	7.50
2	1.63857343	100.0000015	15.00	100.00	7.50
3	1.63857332	100.00	15.00000036	100.00	7.50
4	1.63857338	100.00	15.00	100.0000015	7.50
5	1.63857338	100.00	15.00	100.00	7.50000018
6	0.4270	73.66	19.46	73.66	9.73
.....					
11	0.1279	65.02	23.27	65.02	11.63
.....					
16	0.01145	54.52	27.91	54.52	13.95
.....					
57	0.00829	56.19	30.26	56.19	14.80
.....					
67	0.00663	55.73	29.60	55.73	14.81

Case B : An Initial Guess Of Parameter's Values Deviating By more Than 200% From Their Real Values.					
Iteration No.	Obj. Funct.	K_x[m/day]	K_y[m/day]	α_L[m]	α_T[m]
1	10.6073708	150.00	1.00	150.00	0.500
.....					
9	5.93	57.46	2.01	5746	1.00
10	7.14	22.23	2.39	22.23	1.20
11	5.59	51.74	2.06	51.74	1.03
12	5.51	44.94	2.14	44.94	1.07
.....					
205	0.00756	54.17	30.53	54.17	15.26

Case C : An Initial Guess Of Parameter's Values Deviating Very Far Away From Their Real Values.					
Iteration No.	Obj. Funct.	K_x [m/day]	K_y [m/day]	α_L [m]	α_T [m]
1	6.28570904	1000.00	100.00	1000.00	50.00
.....					
48	2.82	297.77	119.01	297.77	59.51
55	2.81	295.39	118.66	295.39	59.32
.....					
236	0.0157	53.54	32.43	53.54	16.21
.....					
243	0.009	55.68	28.169	55.68	14.08
244	0.0063	55.13	29.44	55.12	14.68
.....					
265	0.0061	54.87	29.87	54.87	14.93
266	0.0006	54.81	29.8	54.81	14.91

Table 1 Case Of Optimisation Of K_x, K_y, α_L and α_T Based On The Objective Function Of Equation(7) With Different Initial Guesses Of Parameters' Values

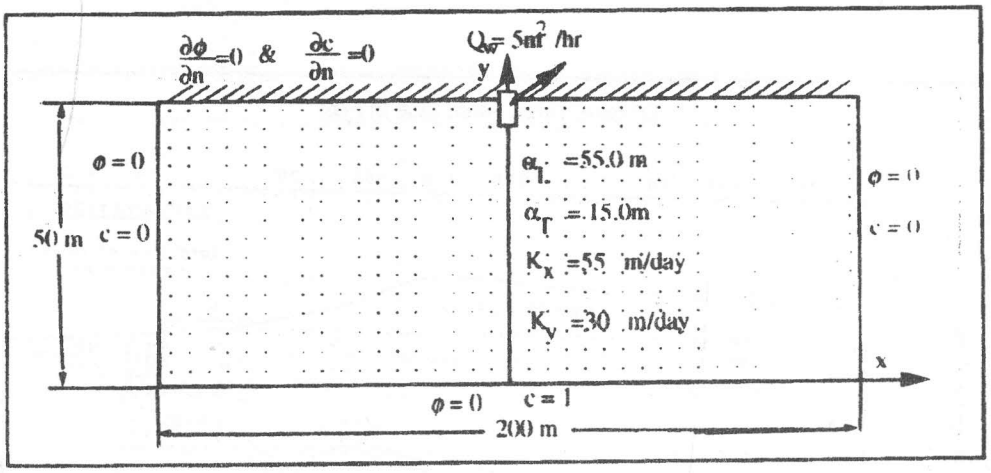

Figure 2. Geometry and boundary conditions for salt water upconing beneath a gallery.

REAL SALT WATER INTRUSION PROBLEM

This problem is based on the Biscayne aquifer in the Cutler area near Miami, Florida. The Biscayne aquifer is a water-table aquifer consisting of solution-riddled limestone and calcareous sandstone extending to a depth of 105 ft below the mean sea level. A cross-section for the area and the chloride concentration map are shown in Figures (3) and (4), respectively. In 1958, samples were collected and pressure heads were measured at a test sites located in the Cutler area[6,7]. This was done before and after a heavy rainfall which sharply increased the elevation of water table. Measurements showed that the distribution of chloride before the recharge pulse could be considered as indicative of steady-state conditions [8].

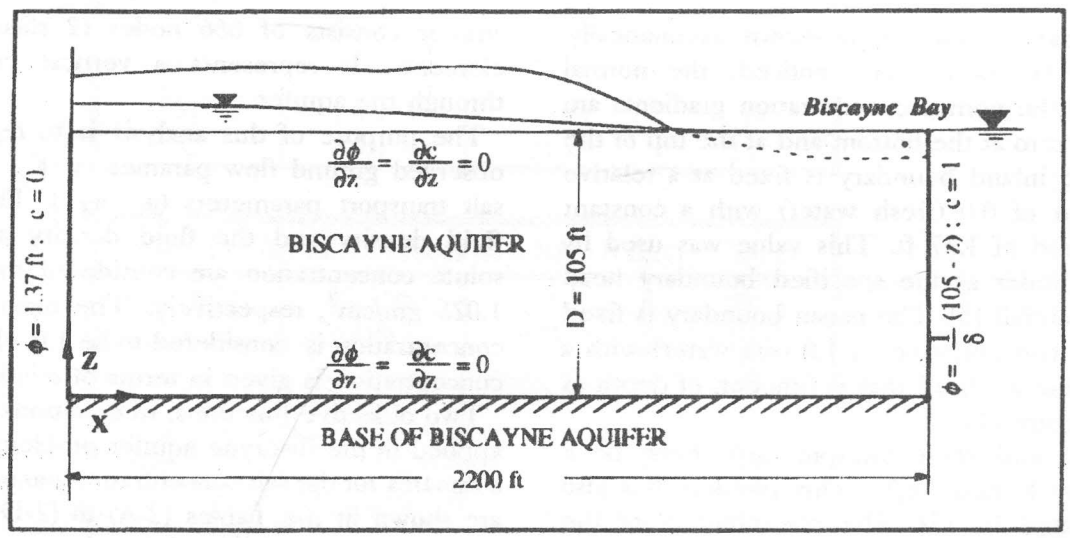

Figure 3. Geometry and boundary conditions for biscayne aquifer problem.

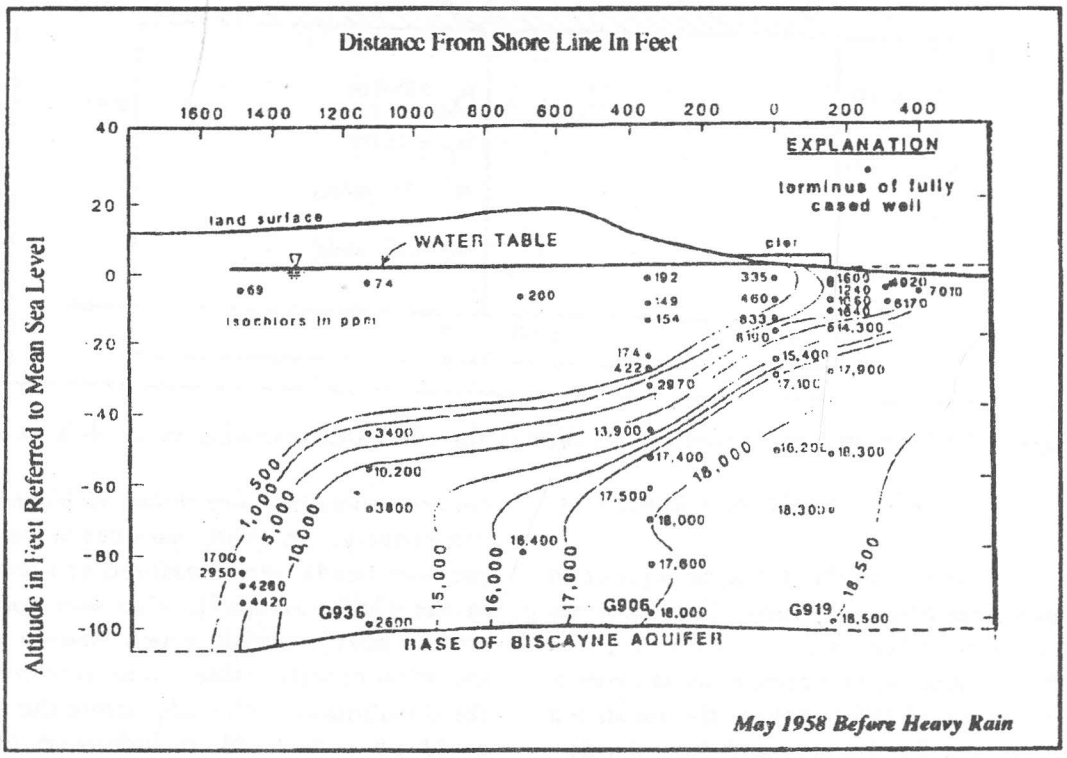

Figure 4. Cross-section through the culter area showing chloride distributions.

The boundary conditions are shown schematically on Figure (3). As may be noticed, the normal velocity and the normal concentration gradients are set equal to zero at the bottom and at the top of the aquifer. The inland boundary is fixed at a relative concentration of 0.0 (fresh water) with a constant hydraulic head of 1.37 ft. This value was used by Segol and Pinder as the specified boundary head before the rainfall [5]. The ocean boundary is fixed at a relative concentration of 1.0 (sea water) with a constant reference head that is function of depth as shown in Figure (3).

Field data and their interpretation have been published by Kohout [6,7]. This problem has also been simulated by [5]. The phenomenon of the circulation of salt, which is clearly noticed in figure (4), means that this is a really good check of the applicability of the automatic calibration protocal.

The simulated domain of interest extends from 600 ft seaward to 1600 ft inland far from the shore line. The used finite element grid for the Biscayne aquifer consists of 666 nodes (2 slices) and 288 elements. It represents a vertical cross section through the aquifer.

The purpose of this analysis is to reproduce the observed ground flow parameters (K_x, K_y) and the salt transport parameters (a_L, a_T). The reference fluid density and the fluid density at maximum solute concentration are considered to be 1.0 and 1.025 gm/cm^3, respectively. The maximum solute concentration is considered to be 1.0, elsewhere the concentration is given in terms of relative values.

Two objective functions, of equations 5 and 7, are applied in the Biscayne aquifer problem. The initial estimates for the salt concentration parameters a_L, a_T are shown in the Tables (2-A) to (2-D) at the first row. In the routine of studying the sensitivity of the objective function to both flow and salt transport parameters, the initial estimates for the flow and salt transport parameters are K_x=3000 ft /day, K_y = 30 ft/day, a_L =70 ft and a_T=20 ft. The results of the optimisation process are given in Table (3).

Case A : An Initial Guess α_L=10.0ft &α_T = 3.0 ft			
Iteration No.	Obj. Funct.	α_L	α_T
1	1.05E-2	10.00	3.0
2	1.05E-2	10.0000012	3.0
3	1.05E-2	10.00	3.0000011
4	4.85E-5	20.9951	2.1445
-	-	-	-
14	4.02E-9	21.85	2.2

Case B : An Initial Guess α_L=150 ft &α_T = 50 ft			
Iteration No.	Obj. Funct.	α_L	α_T
1	0.3075	150.00	50.00
.....			
20	4.25E-5	22.23	0.91
.....			
29	6.97E-9	21.85	2.18

Case C : An Initial Guess α_L=1000 ft &α_T = 300 ft			
Iteration No.	Obj. Funct.	α_L	α_T
1	2.37	1000.00	300.0
.....			
4	2.36E-2	3.33	218.45
.....			
27	2.81E-3	22.88	58.25
28	7.38E-4	23.04	15.57
.....			
41	1.93E-8	21.83	2.19
42	4.02E-9	21.85	2.2

Case D : An Initial Guess α_L=2000 ft &α_T = 700 ft			
Iteration No.	Obj. Funct.	α_L	α_T
1	3.96	2000.00	700.00
.....			
8	4.52E-2	58.57	244.14
.....			
13	1.33E-2	38.77	64.8
.....			
22	2.69E-5	21.21	2.18
-	-	-	-
47	4.57E-9	21.85	2.2

Table 2 Case Of Optimisation Of α_L and α_T Based On The Objective Function Which Is Defined As The Sum Of The Squares Of The Errors In The Salt Concentration Over The Domain With Different Initial Guesses In Case Of A Real Problem.

Iteration No.	Obj. Funct.	K_x[ft/day]	K_y[ft/day]	α_L[ft]	α_T[ft]
1	21.16179920	3000.00	30.00	70.00	20.00
2	21.16179918	3000.000042	30.00	70.00	20.00
3	21.16179921	3000.00	30.000000037	70.00	20.00
4	21.16179931	3000.00	30.00	70.00000126	20.00
5	21.16172005	3000.00	30.00	70.00	20.000000263
6	21.15	7470.97	74.73	69.90	19.98
.....					
16	19.66	11460.17	120.49	57.37	17.55
.....					
42	15.59	10556.86	122.07	35.87	12.65
.....					
68	15.59433815	6587.54	76.18	35.86	12.65
69	15.59433816	6587.54	76.17	35.86	12.65
70	15.59433833	6587.54	76.17	35.86	12.65
71	15.59433814	6587.58	76.17	35.86	12.65
72	15.59433815	6587.62	76.18	35.85	12.65
73	15.59396279	6587.52	76.18	35.85	12.66
74.	15.59396280	6587.48	76.18	35.85	12.66
75	15.50250148	10541.36	122.10	35.57	12.56
76	15.50250148	10541.36	122.10	35.65	12.56
77	15.52250149	9441.47.	109.32	35.65	12.59
78	15.50250152	10541.35	122.10	35.57	12.56
79	15.50250149	10541.36	122.10	35.57	12.56
80	15.50250148	10541.36	122.10	35.57	12.56
81	15.50250148	10541.36	122.10	35.57	12.56
.....					
96	12.51	13900.53	169.12	27.40	9.97
.....					
117	11.18	14892.08	167.39	25.25	8.99
118	11.18	14892.08	167.39	25.25	8.99
119	11.18	14892.08	167.39	25.25	8.99
.....					
127	11.18	10829.47	121.7	25.22	8.99
128	11.18	10829.47	121.7	25.22	8.99
.....					
133	10.81	7090.06	75.33	25.22	8.75
.....					
143	10.66	2922.59	29.88	25.13	8.66
144	10.66	2922.59	29.88	25.13	8.66
145	10.66	2922.59	29.88	25.13	8.66
.....					
156	10.65	2829.18	28.07	25.12	8.59
.....					
217	4.91	9795.53	12.74	25.45	5.65
.....					
243	4.89	19473.15	25.33	25.45	5.64
244	0.61	20271.83	28.15	25.02	3.03
245	0.57	20271.83	28.14	25.02	3.03
.....					
334	0.00115	1278.67	2.567	21.87	2.194

Table 3 Case Of Optimisation Of K_x, K_y, α_L and α_T Based On The Objective Function Which Is Defined As The Sum Of The Squares Of The Errors In The Potential And The Salt Concentration Over The Domain With An Initial Guess Of Parameter Values Differing By More Than 100% From Their Real Values.

It is observed from tables 2-A, 2-B, 2-C and 2-D that the objective function defined by equation (5) is decreasing. The required number of iterations is dependent upon the value of initial guess as expected. These tables show that the number of iterations increases as the initial guess deviates from the real value, but not in the same rate. When the initial guess is increased relatively to very high values the iteration procedure converges fast to lower values then it converges slower to the real value. The initial guess value of a_L is increased up to about 100 times its real value while the initial guess value of a_T is increased up to about 300 times its real value.

Table (3) shows the effect of changing the flow parameters K_x and K_y on the objective function [9]. The objective function is defined here as the sum of the squares of the errors in the potential and the salt concentration over the domain. It is clear that these parameters are more significant in increasing the objective function compared to salt transport parameters a_L and a_T. The number of iterations jumps to 344 iteration due to increasing the initial guess of K_x to about twice its real value, and K_y to about 15 times its real value[9].

CONCLUSION

A new scheme for indirect calibration is developed. This scheme has the advantage of calibrating the three dimensional model to calculate the flow and salt transport parameters based on a converging protocol regardless of the initial guess for these parameters. It is concluded that field tests are very helpful to start with a reasonable initial guesses which are important in accelerating iteration procedure, therefore, saving CPU time. One of the major conclusions is that the three dimensional model is more sensitive to flow parameters rather than salt transport parameters. An accurate initial guess for initial flow parameters is much more important than the initial guess for salt transport parameters since flow parameters are implicitly effective in salt transport equation.

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