Journal of Hydrology, 69 (1984) 197—222
Elsevier Science Publishers BV, Amsterdam — Printed in The Netherlands

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GROUNDWATER-FLOW PARAMETER ESTIMATION AND QUALITY MODELING OF THE EQUUS BEDS AQUIFER IN KANSAS, U.S.A.

MARIOS A. SOPHOCLEOUS

Kansas Geological Survey, University of Kansas, Lawrence, KS 66044 (U.S.A.)

(Received February 3, 1983; revised and accepted May 23, 1983)

ABSTRACT

Sophocleous, M.A., 1984. Groundwater-flow parameter estimation and quality modeling of the Equus Beds aquifer in Kansas, U.S.A. J. Hydrol., 69: 197—222.

The salinity problems created in the Burrton area as a result of poor oil-field brine disposal practices of the past continue to be a major concern to the area depending on the Equus Beds aquifer for water, including the City of Wichita, Kansas. In this paper, an attempt is made to predict where and how fast the brine plume will move in this area, and what the average chloride concentrations in different parts of the aquifer are. In order to make such predictions, it was necessary to get a calibrated model of the groundwater-flow velocity field. Multiple regression analysis is used for parameter estimation of the steady-state groundwater-flow equation applied in the most critical area of the Equus Beds aquifer. Results of such an analysis produced a correlation coefficient of 0.992 between calculated and observed values of hydraulic head. A chloride transport modeling effort is then carried out despite some serious data deficiencies, the significance of which are evaluated through sensitivity analysis. Thus, starting with the quasi steady-state conditions of the early 1940's, it was possible to match the present chloride distribution satisfactorily. Chloride concentration predictions made for the year 2000 indicate that the quality of the Wichita well-field waters will not generally deteriorate from their present condition by that time.

STATEMENT OF THE PROBLEM

In recent years it has become clear that the groundwater quality in parts of the Equus Beds aquifer, which approximately coincides with the boundaries of the Equus Beds Groundwater Management District (Fig. 1), is progressively deteriorating. Farmers are noticing that their water is becoming salty and some have had to abandon their wells. Because of salinity problems, the City of Burrton found it necessary to construct a new supply well in 1972 ~ 3 km north of its original location.

The source of this saline water is generally believed to be oil-field brine that leaked from surface disposal ponds during the early history of oil and gas development in the area, mainly during the 1930's and 1940's (Williams and Lohman, 1949; Latta, 1963; Leonard and Kleinschmidt,

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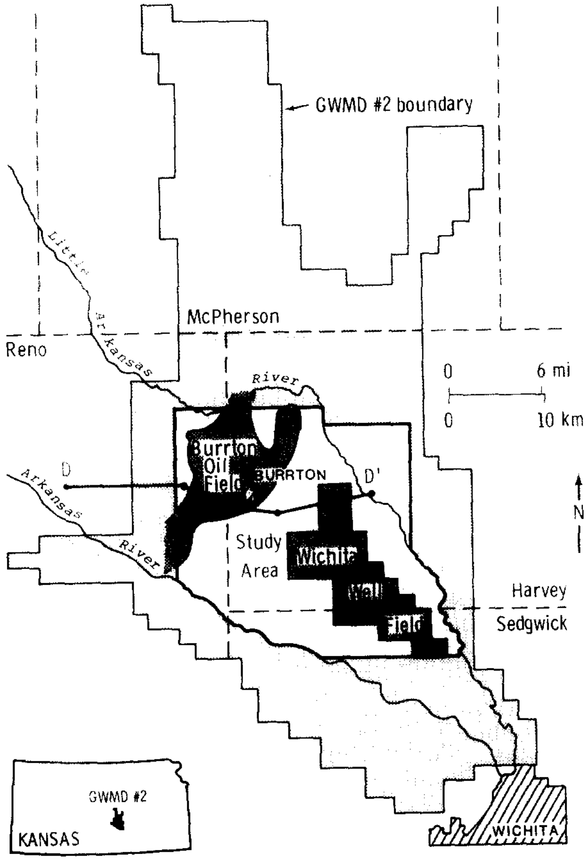

Fig. 1. Equus Beds aquifer as indicated by the boundaries of the Equus Beds Groundwater Management District, and study area.

1976). Locally, pollution by saline water may also have been caused by upwelling of oil-field brine injected under pressure into the so-called "lost circulation zone" corresponding to the Hutchinson Salt Member of the Permian Wellington Formation underlying the Equus Beds aquifer, and possibly by leakage of brine from corroded or improperly-cased saltwater disposal wells or old abandoned oil wells. Initiation of water-flood operations for secondary recovery in oil fields of the Equus Beds area has provided yet another potential mechanism for brine contamination of the freshwater aquifer.

The salinity problem created in the Burrton area continues to be a major concern in the operation of wells in the Wichita well-field region (Fig. 1), which supplies water for the municipal and industrial needs of the City of Wichita. At present, both the City of Wichita and the Equus Beds

Groundwater Management District maintain chloride monitoring programs for observation wells in the vicinity of Burrton and the Wichita well field.

Localized deterioration of groundwater quality in the Burrton area through intrusion of brine solutions is suggested by concurrent increases in sodium and chloride concentrations and specific conductance values above regional background levels (Hathaway et al., 1981). The affected wells appear to be underlain by the eastern margin of the Hutchinson Salt Member of the Wellington Formation (lost circulation zone), as can be seen in section *DD'* (Fig. 2), and are in the proximity of oil fields, both of which are sources of brine.

Groundwaters from the Equus Beds aquifer normally contain $< 100\,\mathrm{mg\,l^{-1}}$ of chloride ions; therefore, higher concentrations commonly indicate the presence of a brine pollutant. However, chloride values by themselves do not serve to distinguish between the two above-mentioned potential sources of brine pollution in the area. Geochemical evidence based primarily on Br/Cl ratios and supported by Na/Cl and I/Cl ratios indicate that the main source of salinity in the area is oil-field brine (Leonard and Kleinschmidt, 1976; Hathaway et al., 1981; Sophocleous, 1982; Whittemore and Basel, 1982).

In assessing the significance of groundwater contamination, one of the most difficult problems is predicting the degree and extent of contamination. This problem arises because of the complex array of factors influencing the dispersal of the contaminant in the subsurface. In spite of considerable progress, much of our present understanding is still limited

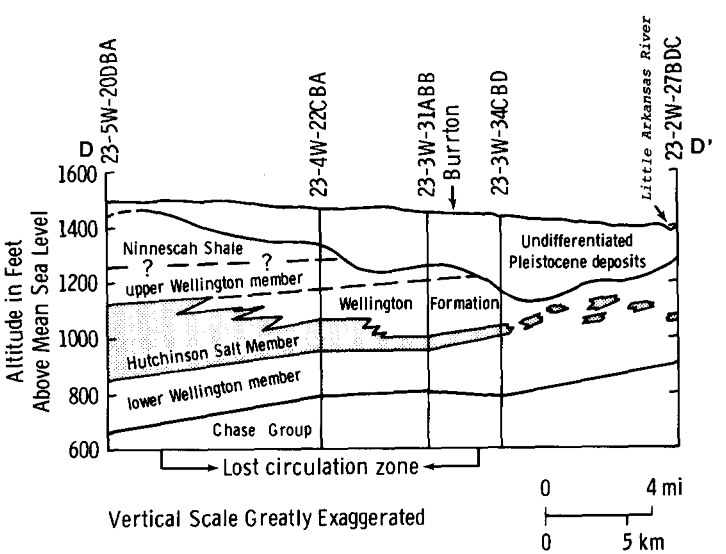

Fig. 2. Geologic cross-section in the vicinity of Burrton. To convert values in feet to values in meters, multiply by 0.305 (adapted from Gogel, 1981).

and largely empirical. However, the success in recent years of sophisticated techniques for the mathematical description and predictive analysis of groundwater systems has provided the impetus to develop elaborate mass-transport models. Nevertheless, the application of such methodologies to field situations is not straightforward. The acquisition of reliable data seems to be a critical limiting factor in the application of such models to field situations, in addition to the requirement of acquiring enough such data for the verification of these models.

The purpose of this study is to attempt in a general way to answer the following questions for the Burrton area: (a) can we predict where and how fast the brine plume will move?, and (b) can we predict the average concentration of a contaminant in different areas of a flow system influenced by several contaminant sources as is the case for the study area? The first question could be answered using groundwater-flow models alone. However, in order to answer the second question, a flow model must be coupled to a water-quality model. Therefore, we decided to run a solute transport model using the conservative chloride solute as the indicator of brine encroachment in the study area. It should be stressed at the outset that this effort should be regarded only as a "first-approximation" attempt to answer the previously posed questions because of considerable data deficiencies, as will be mentioned further on.

GROUNDWATER-FLOW MODELING RATIONALE

In a groundwater system, two processes are responsible for the physical transport of mass from one point to another: convection and dispersion. Chemical and biological processes may act in addition to the physical transport processes. However, convective transport is the primary transport mechanism that determines the extent of pollutant travel from the site of mass entry to the system. The direction and velocity of pollutant transport generally is assumed to be identical to that of the groundwater. Therefore, a thorough understanding of the hydrogeological setting and especially of the aquifer flow field is essential because an accurate prediction of solute transport cannot be made without first fully understanding the fluid flow system. Models of pollutant transport inevitably include a model of groundwater flow.

An area of the Equus Beds aquifer was selected for the purpose of understanding such features of the hydrogeologic setting as water-table configuration, hydraulic conductivity distribution, and boundary fluxes, which control the pattern of groundwater flow and hence also control the pattern of convective transport. The area selected for this purpose is a 622-km^2 area in the vicinity of Burrton, where most of the groundwater pollution took place in the past (Fig. 1) and where there is a denser network of observation wells than in other parts of the aquifer.

Since the selected model area does not encompass the entire Equus Beds aquifer and its natural boundaries, it is important that meaningful boundary conditions be applied to the selected area. For this purpose, a number of maps of the area were compiled indicating water-table and bedrock configurations, saturated thickness, depth to water table, and water-level declines since the early 1940's. A study of these maps and particularly of the water-level decline map indicated that the proposed study area has been enclosed by a zero water-level decline since 1940 (Fig. 3). Because of this and of the existence of the two major streams enclosing parts of the study area, it seemed reasonable to employ specified hydraulic-head boundary conditions along the boundaries of the area. The Arkansas River, the largest stream, is used as a constant-head boundary in the south-western boundary of the study area, while the Little Arkansas River is considered as a constant-head boundary at the southeastern boundary of

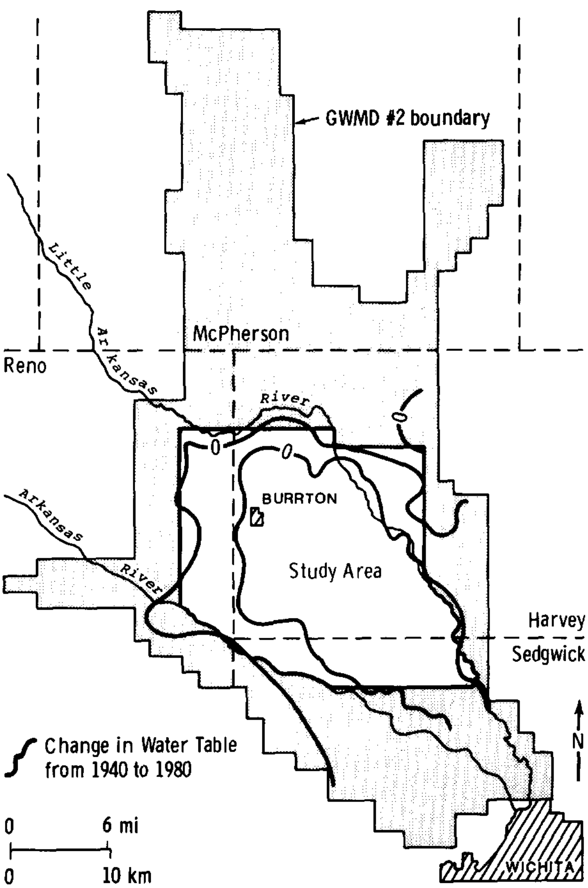

Fig. 3. 1940—1980 zero water-level decline contours for the study area.

the study area, after the contributions of Kisiwa, Emma and Sand Creeks are added to the Little Arkansas River. Therefore, a constant-head boundary condition was employed for all boundaries of the selected area.

Since the scope of this project is not to engage in a detailed transient-flow simulation where all irrigation, municipal and industrial pumpages must be compiled and checked for each year since records have been kept, it was decided that the area's steady-state velocity field that has existed since the early 1940's would still be a satisfactory approximate flow distribution, especially since the area has not yet experienced any serious water-level-decline problems. This assumption will constitute significant saving of modeling costs and human effort in a transient solute-transport simulation. Thus, once the flow field is determined, it remains constant through time, and in a transient mass-transport simulation we can examine how the pollutants are spreading in space and time given that average flow velocity field.

HYDROGEOLOGIC SETTING OF THE CASE STUDY

The study area consists of unconsolidated deposits of Pleistocene age in the upper part and Pliocene age in the lower part (Stramel, 1967) overlying the bedrock, which consists of consolidated Permian rocks (Wellington Formation and Ninnescah Shale). The Wellington Formation (Fig. 2), which is the predominant bedrock unit in the study area, can be divided (Leonard and Kleinschmidt, 1976; Gogel, 1981) into an upper member consisting mainly of shale with minor amounts of gypsum, anhydrite, dolomite and siltstone; a middle unit which, in the western part of the study area, is the Hutchinson Salt Member consisting of salt interbedded with minor amounts of shale, gypsum and anhydrite; and a lower member consisting mostly of anhydrite and gypsum, with some thin beds of shale and dolomite. The unconsolidated rocks, of fluvial origin, consist of gravel, sand, silt and clay in various proportions. The sand and gravel beds generally lie between lenses of silt, clay and sandy clay. For the most part, the fluvial deposits are buried beneath a mantle of wind-deposited sand, silt and clay. A large area of sand dunes, mostly underlain by discontinuous clay lenses, exists north of Burrton (Fig. 4). The steady-state water-table configuration which is not much different from the present water-table configuration is also shown in Fig. 4. The Equus Beds aquifer is recharged principally from precipitation, which averages $\sim 76\,\mathrm{cm\,yr.}^{-1}$. It is widely believed (Williams and Lohman, 1949; Stramel, 1967) that the sand-dune area in the northwestern part of the study area absorbs most of the precipitation that falls and contributes appreciable quantities of water to the aquifer. The two major streams of the area, the Arkansas River and the Little Arkansas River, form parts of the boundary of the study area. Detailed descriptions of the geology and hydrogeology of the area are given by

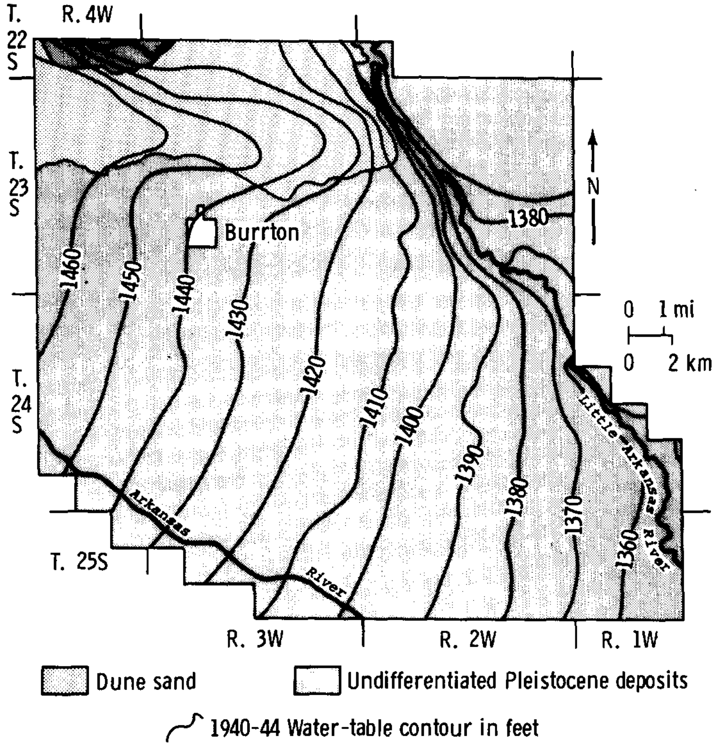

Fig. 4. Surficial geology and 1940—1944 water-table configuration.

Williams and Lohman (1949), Stramel (1956, 1967), Petri et al. (1964), Albert and Stramel (1966), and Pinney et al. (1975).

MODEL CONSTRUCTION

Special emphasis is given in this phase of the study to obtaining a calibrated model of the groundwater flow field. Groundwater models are often difficult to apply under realistic field conditions because of a lack of sufficient information about the parameters entering into the model. It is rare that parameter data estimated or measured in the field or laboratory, are either reliable or complete enough to employ directly in a model to reproduce estimated head data with an acceptable model fit. The question then arises as to whether there is an indirect way of supplementing the information about the parameters, by analyzing the response of the flow system to certain fully or partially known inputs. The problem of determining an optimal set of parameters for a model, given some prior information about the system and its behaviour, is often referred to as the calibration, parameter estimation or inverse problem. As a result of model calibration, adjustment of parameter values, and sometimes of basic model structure, is used to improve model fit. There are two basic groups of methods currently in use to accomplish this:

(1) Trial-and-error procedures for which there is no methodology that guarantees that the simulations will proceed in a direction that could lead to the best set of parameters; this process is often time consuming and expensive and sometimes can result in no answer.

(2) Optimization methods involving minimizing an objective function. This process allows a determination of the optimum set of parameters and predicted heads whenever such an optimum exists. Furthermore, analysis of the results obtained from an optimization procedure permits determination of model and parameter reliability as well as the best model to use among several alternative possibilities.

The methodology selected for this study is that of *multiple regression*. The objective of multiple regression is to find the parameters of a given model that produce the best fit of the calculated dependent variable, head in our case, to the observed dependent variable, then assess the significance of the fit and the reliability of the model and predictions to be made with it. This is also the objective of most modeling studies and suggests that classical multiple-regression procedures could be adapted to such studies.

The calibration or parameter estimation problem may be viewed as a classical nonlinear regression problem with a solution of the appropriate flow equation forming the regression equation and all unknown quantities such as hydrogeologic parameters, sources, sinks and boundary fluxes forming the parameters. The set of *measured* hydraulic heads are observations of the dependent variable for which a set of least-squares estimates is to be obtained. This viewpoint not only has the advantage of answering the problems involving the contouring of head data, but also allows implementation of many of the various methods and tests that have been developed to analyze regression problems (Cooley, 1977).

THE REGRESSION PROBLEM

The approximate general equation governing steady-state groundwater flow in two dimensions, which is to be fitted to the observed head data, is:

$$\frac{\partial}{\partial x_i}\left(T_{ij}\frac{\partial h}{\partial x_j}\right) + R(H-h) + W = 0 \tag{1}$$

where for areal flow T_{ij} is the transmissivity tensor $[L^2\ T^{-1}]$; R is the hydraulic conductance or *leakance* (hydraulic conductivity divided by thickness) of sediments underlying a stream or of an aquitard underlying or overlying the aquifer $[T^{-1}]$; W is the source-sink strength (positive for a source) $[\mathrm{L\,T^{-1}}]$; this term is composed of an areally distributed part and a point-function for pumping wells; h is the hydraulic head in the aquifer [L]; H is the head at the stream bottom or at the distal side of the aquitard [L]; and x_i is a Cartesian coordinate system [L].

To approximate the variability of a given parameter, the region of interest is subdivided into a number of zones in which the parameter is assumed to be constant within each zone. Zones of one type of parameter, such as transmissivity, do not necessarily correspond to zones of another type, such as recharge.

For most field problems eq. 1 with its attendant boundary conditions cannot be solved analytically. Thus, the regression solution must be based on a numerical solution of eq. 1, which is expressed as a matrix equation. For the present study, the solution is obtained by using the integrated finite-difference method.

In matrix form the numerical solution to eq. 1 (Cooley, 1977, 1979) is given as:

$$\underline{D}\underline{h}_m = \underline{q} \tag{2}$$

where $\underline{D}$ is the square coefficient matrix of order m, the number of nodes used to discretize the modeled region involving parameters T_{ij} and R; $\underline{h}_m$ is the hydraulic head vector of order m; and $\underline{q}$ is the known vector of order m, involving source-sink terms, W, specified head, h_{B}, and boundary flux, q_{B}, values.

The set of optimal parameters is defined as the set that minimizes the objective function:

$$S = \underline{e}^{\mathrm{T}}\underline{w}\underline{e} = (\underline{h}^{\mathrm{obs}} - \underline{h})^{\mathrm{T}}\underline{w}(\underline{h}^{\mathrm{obs}} - \underline{h}) \tag{3}$$

where $\underline{h}^{\mathrm{obs}}$ is the vector of observed heads; $\underline{h}$ is a vector of predicted heads; $\underline{e} = \underline{h}^{\mathrm{obs}} - \underline{h}$ is the residual vector consisting of the deviations of calculated heads from observed heads; superscript T indicates transpose; and $\underline{w}$ is a diagonal weight matrix ranging from 0 to 1 that describes the reliability of h^{obs} at each node. If for observation l, $w_l = 0$, then there is no observed head at that node. S is the weighted sum of squared deviations of calculated heads from observed heads, which is to be minimized. The use of the above objective function is equivalent to minimizing the error variance.

If the parameters to be computed (such as all the different values of T_{xx}, T_{yy}, R, W and q_{B}) are designated as vector $\underline{b}$, then the normal equations derived by minimizing eq. 3 with respect to each parameter may be written as:

$$\underline{e}^{\mathrm{T}}\underline{w}(\partial\underline{e}/\partial\underline{b}) = 0 \tag{4}$$

Cooley (1977) derived an iteration technique whereby the necessary elements of $\underline{e}$ and their derivatives are obtained through use of a modified Gauss—Newton linearization scheme applied to eq. 2. The technique yields a regression equation, which upon convergence of the procedure may be written as:

$$\underset{\sim}{h}^{n+1} - \underset{\sim}{h}^{n} = \underset{\sim}{X}^{n} (\underset{\sim}{b}^{n+1} - \underset{\sim}{b}^{n}) \tag{5}$$

where $\underset{\sim}{X}^n$ is a sensitivity matrix $\partial h^n / \partial b_j$; n is the iteration number; and $j = 1, 2, \ldots, p$ (p = number of parameters). The sensitivity coefficients X_{ij}, or simply sensitivities, indicate the change in the value of head h_i for a unit change in parameter b_j. The regression algorithm (Cooley, 1977) uses only observed values of head in the criterion S for the best-fit solutions. If data are available as prior information on the parameters, these are added to the algorithm.

ASSUMPTIONS FOR THE REGRESSION ANALYSIS

The nonlinear model — assumed to be the true model — represented by the solution of eq. 2 for $\underset{\sim}{h}$, which is the subset of $\underset{\sim}{h}_m$ applying at nodes that are observation nodes, can be written for observation l as:

$$h_l^{\text{obs}} = f(\xi_l, \beta) + \epsilon_l \tag{6}$$

where f indicates a function that is the solution of eq. 2; ξ_l is a vector of independent variables that is an undetermined but observable function of coordinates x, y, the problem geometry and boundary conditions; β is the vector of true parameters; and ϵ_l is an error in observation of head.

In order to analyze statistically the results of and the predictions made by the regression model, it is assumed (Draper and Smith, 1980) that:

$$\mathrm{E}(\epsilon_l) = 0 \tag{7}$$

$$\mathrm{Var}(\epsilon_l) = \sigma^2 \tag{8}$$

$$\mathrm{Cov}(\epsilon_l, \epsilon_m) = 0, \quad l \neq m \tag{9}$$

where E, Var and Cov are the expected value, variance and covariance operators respectively. These assumptions indicate that ϵ_l is considered to be a random variable with zero mean and constant variance σ^2 and that ϵ_l and ϵ_m ($l \neq m$) are uncorrelated. In addition, it is often assumed that ϵ_l is normally distributed with mean 0 and variance σ^2; this means that the elements of ϵ are independent as well as uncorrelated and allows the use of statistical tests and measures involving the F and t distributions (Draper and Smith, 1980).

Because β is unknown, ϵ is not observable, and the assumptions given above cannot be checked directly. However, they may often be checked indirectly, after the regression and model analysis have been performed.

MODEL IMPLEMENTATION

The location of the 78 observation wells used for this study is given in Fig. 5. These wells were selected because they happened to fall at the nodes of the two-dimensional model grid network consisting of 2.6-km^2 blocks or were located very near to them (generally less than 0.4 km from a node). As a result of the employment of this regular finite-difference grid, a small number of wells had to be omitted in order to remain true to our claim of using "measured" head values at the appropriate node. A finite-element model such as the one employed by Cooley (1977) would have eliminated this shortcoming. Such a large grid spacing is used because the scope of this study is for generalized, approximate analysis. In order to reduce the number of parameters to be estimated, the method of parameter zonation is employed. Such parameter zonation, shown in Fig. 5, is based on the geology of the area, its transmissivity distribution as presented by Richards and Dunaway (1972) and Green and Pogge (1973), and other evidence for recharge variability, such as the water-table configuration. Preliminary runs using different zonations confirmed that the currently considered

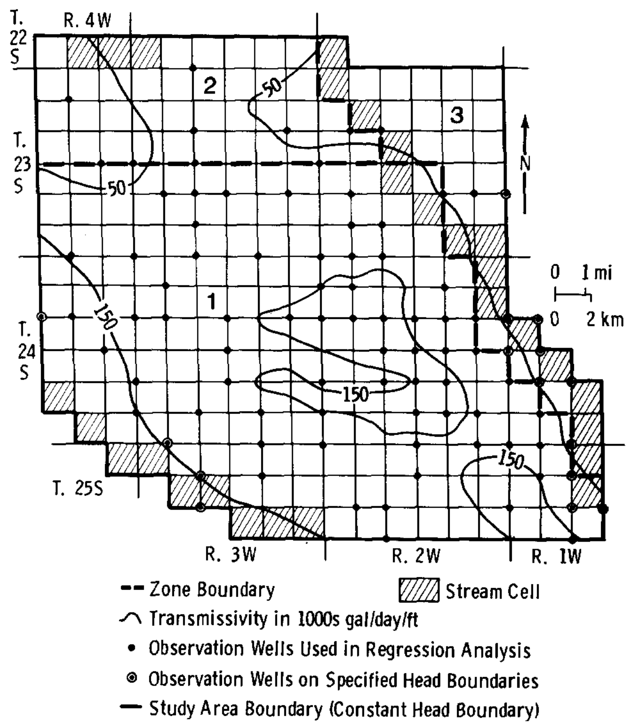

Fig. 5. Location of observation wells and hydrogeologic zonation in the study area. To convert transmissivity contours in 1000's gal. $day^{-1} ft.^{-1}$ to $m^2 day^{-1}$, multiply by 12.42.

zonation is satisfactory since it resulted in the best fit between observations and calculated head values. Parameters used for the study area are transmissivity (considered to be isotropic), areal recharge, leakance of the stream beds, and the specified head boundary at the southern part of the study area. Seepage data employed in calculating leakance were available only for the Little Arkansas River, but were assumed to be representative of the Arkansas River as well. Each parameter is considered constant within a zone. It should be stressed that such constant-parameter zonation is probably an oversimplification of reality, given the highly heterogeneous nature of the Equus Beds deposits.

Transmissivity is considered constant for zones *2* and *3* (Fig. 5), while recharge is allowed to differ. Transmissivity for zone *1*, which encompasses the most productive part of the Equus Beds aquifer, is much higher than for zones *2* and *3* (refer to data by Richards and Dunaway (1972), a portion of which are shown as transmissivity contours in Fig. 5), while recharge for zone *2*, which coincides with the sand-dune area, is much higher than recharge for zones *1* and *3*, both of which are considered to have the same recharge value, based on similar soil and topographic conditions. Because of the lack of sufficient data, leakance of sediments underlying the major streams of the area is considered constant for all zones. It should be noted that the cells of the finite-difference grid for streams have much larger area than the surface areas of stream segments in them; therefore, the model leakance parameters should be considered effective values. The values of specified hydraulic head along the boundaries were estimated from the 1940—1944 water-table map of Williams and Lohman (1949).

MODEL ANALYSIS

Results of the analysis, which used equal weights (reliabilities) for all observation wells, are shown in Table I. From that table, the fit of calculated to observed values of head is very good, as indicated by the high value of the correlation coefficient $R = 0.9920$. The value of the ratio of the square root of the error variance over the difference between the highest and the lowest value of head in the region, $s/\Delta h$, is $1.1/44.8 = 0.0245$, a relatively small value, so that errors in the model are considerably smaller than the variation in the model response as indicated by the maximum head loss $\Delta h = 44.8$ m.

The standard error of the estimate is a measure of the range over which the respective parameters may be varied and produce a similar solution for the dependent variable as that obtained using the estimated parameter. The standard error of the estimate for the *i*th parameter is given by the square root of the *i*th diagonal component of the variance—covariance matrix $(\underset{\sim}{X}^{\mathrm{T}} \underset{\sim}{w} \underset{\sim}{X})^{-1} s^2$, where s^2 is the sample error variance. Examination of Table I indicates that the standard errors for the parameters are generally

TABLE I

Summary of parameter estimation results for the Equus Beds aquifer

Zone	Transmissivity (m^2 day^{-1})	Standard error (m^2 day^{-1})	Recharge (10^{-4} m day^{-1})	Standard error (10^{-5} m day^{-1})	Leakance (10^{-4} day^{-1})	Standard error (10^{-4} day^{-1})
1	2,917	711	1.151	3.536	4.483	1.144
2	247	58	4.456	8.553	4.483	1.144
3	247	58	1.151	3.536	4.483	1.144

Square root of error variance, $s(m)$: 1.111; correlation coefficient, R: 0.9920.
Estimated specified heads of the first and last nodes in a sequence along the bottom specified-head boundary of the study area with their standard errors in parentheses (m): 423.5 (0.88), 413.6 (1.00).

< 25% of the magnitude of the respective parameters. Comparison of the estimated sum of squared errors or error variance obtained using these parameter estimates (Table I) to the error variance obtained using the prior estimates (Table II) shows an error variance reduction of > 57.2% as a result of the parameter estimation procedure. The resulting flow velocity field is shown on Fig. 6.

TABLE II

Prior estimates of regression parameters for the Equus Beds case study*

Zone	Transmissivity (m^2 day^{-1})	Recharge (10^{-4} m day^{-1})	Leakance (10^{-3} day^{-1})
1	1652	2.09	6.5
2	609	3.47	6.5
3	609	2.09	6.5

*Averaged values from Richards and Dunaway (1972), Green and Pogge (1973) and other sources.

In this study, prior estimates of such model parameters as transmissivities, recharge and leakance values are included in the regression analysis as prior information (Table II). In cases where an attempt is made to find all model parameters in the absence of measured flow rates, singularity of the least-squares coefficient matrix can occur, resulting from employing the previously-mentioned multiple-regression procedure. In such cases, the singularity problem can be rectified by using prior information. Also, in cases

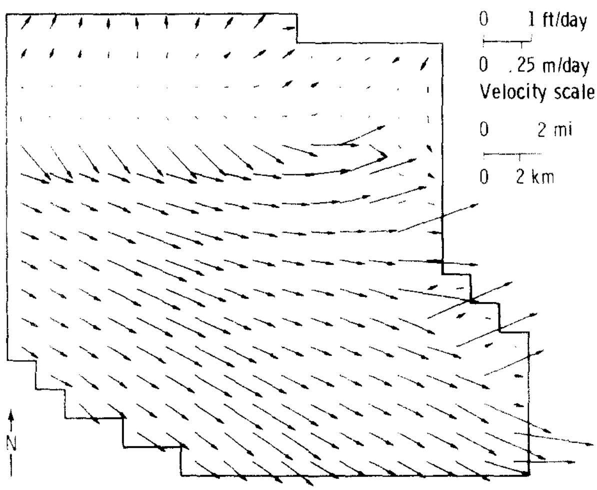

Fig. 6. Groundwater-flow velocity field in the study area.

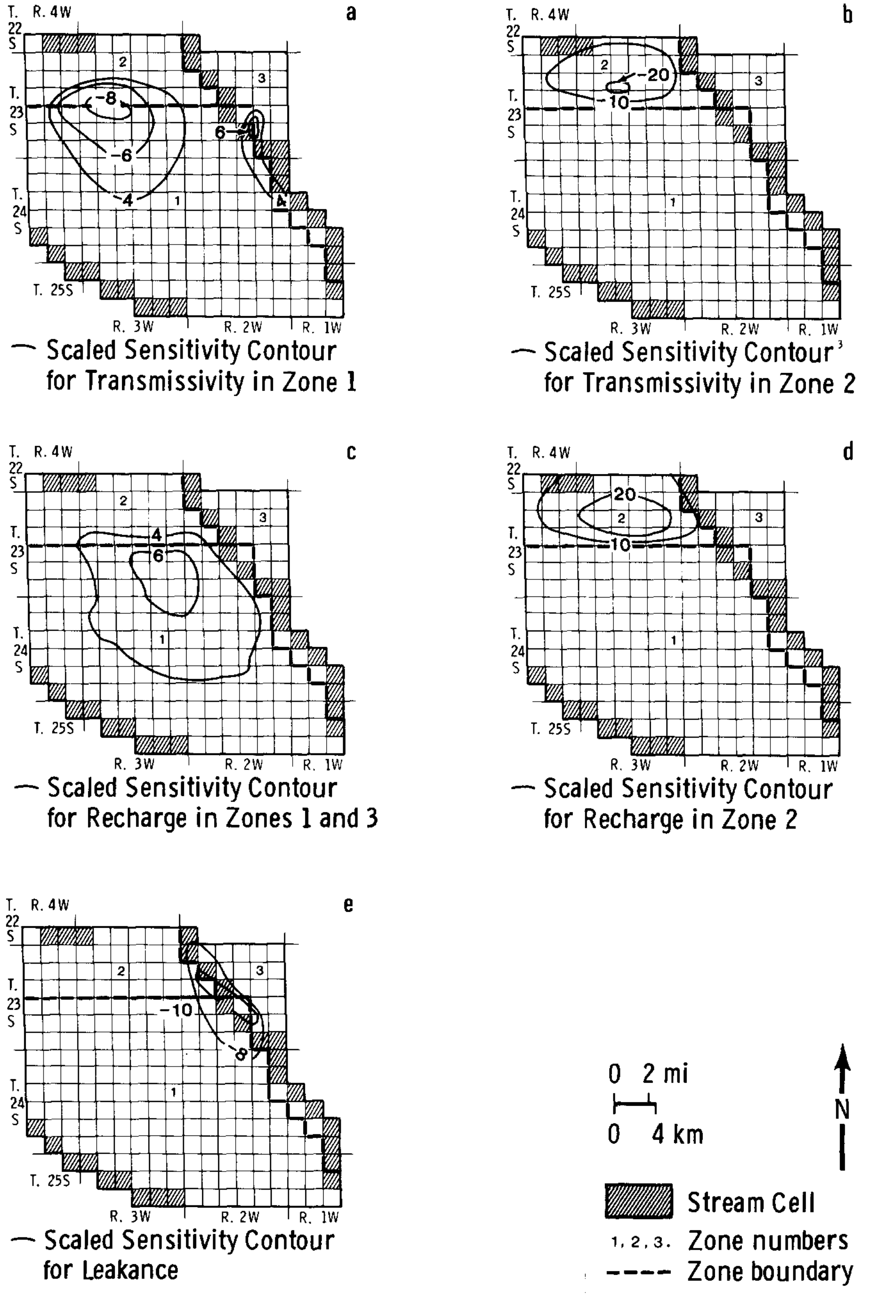

Fig. 7. Scaled sensitivity contours for transmissivity (a and b), recharge (c and d), and stream leakance (e).

where the only source of singularity is that a column of the sensitivity matrix $\underset{\sim}{X}_j = 0$, then prior information on parameter j will rectify the problem (Cooley, 1982). The variability of such prior information is represented in this model by a coefficient of variation. However, because of the small sample size of such information or the crude nature of its estimation, we decided to adjust the coefficients of variation based on how representative we felt the values are compared to the overall hydrogeologic analysis of the Equus Beds aquifer. In general, we found that by adjusting the coefficients of variation on a trial-and-error basis within limits, we were able to obtain a better fit between observed and calculated head values, although this procedure renders the model more approximate.

Fig. 7 shows plots of the scaled sensitivities, $\underset{\sim}{Z}$, of the head distribution with respect to the recharge, transmissivity and leakance parameters for all three zones. The scaled sensitivities, $\underset{\sim}{Z}$, are sensitivities scaled with respect to the parameters, that is:

$$\underset{\sim}{Z} = \underset{\sim}{X} \cdot \underset{\sim}{B} \qquad \text{where} \qquad \underset{\sim}{B} = \mathrm{diag}\,(b_1, b_2, \ldots, b_p)$$

The computed head distribution is least sensitive to transmissivity and recharge for zones *1* and *3* (Fig. 7a and c). The values of recharge are relatively small in those zones, and any small curvature of the potentiometric surface in these zones may be obscured by irregularities in the measured water-level data. The solution for head distribution is most sensitive to recharge and transmissivity for zone *2* (Fig. 7d and b), where recharge and hydraulic gradients are both high. The head distribution is also relatively sensitive to the leakance value (Fig. 7e). It should be noted that the plot of scaled sensitivities for leakance indicates only that portion of the streams enclosing the study area that is not considered to be of the Dirichlet type of boundary. Examination of Fig. 7 shows that there is a considerable variation in sensitivity, indicating that additional data points in high-sensitivity areas would improve model results.

Residuals produced by the model were analyzed in order to examine the possibility that the various assumptions concerning their distribution had been violated. Aspects that could be investigated include evidence for spatial nonrandomness and evidence that the disturbances are not approximately normally distributed. Draper and Smith (1980) give a number of methods for examining residuals and they emphasize that graphical procedures involving visual analysis are very valuable tools for detecting nonrandomness, because violations of assumptions serious enough to require corrective action generally are apparent on the various plots. Residuals were thus examined and showed no evidence of spatial non-randomness or non-normality (Sophocleous, 1982).

MASS-TRANSPORT MODELING — BASIC DATA DEFICIENCIES

Once the groundwater-flow model was obtained and calibrated, the next step was the formulation of a mass-transport model. As was mentioned previously, however, serious data deficiencies were experienced during this mass-transport modeling phase of the study. Preliminary evaluation of the chemical-quality data revealed that a comprehensive description of water quality in the aquifer would be very difficult because of the manner in which water samples were collected for analysis (Leonard and Kleinschmidt, 1976). For example, analyses were erratically distributed in time and space; methods of collection and analysis of the samples varied widely; many sampling locations were poorly or inaccurately recorded; and the depth of the zones sampled were poorly defined. Not until the recent establishment of the salt water-monitoring well network by the Equus Beds Groundwater Management District could definite chloride patterns be easily recognized in the area.

The sources and rates of brine entry into the groundwater flow system are not well understood. However, an unpublished map of old surface disposal ponds with an approximate average rate of brine disposal was obtained from the Kansas Department of Health and Environment (R. O'Connor, pers. commun., 1982). This map was verified and supplemented by studying old aerial photos of the area and identifying the disposal ponds. Fig. 8 shows the general area of major concentration of disposal ponds, although such ponds also existed to the north of the indicated area. In

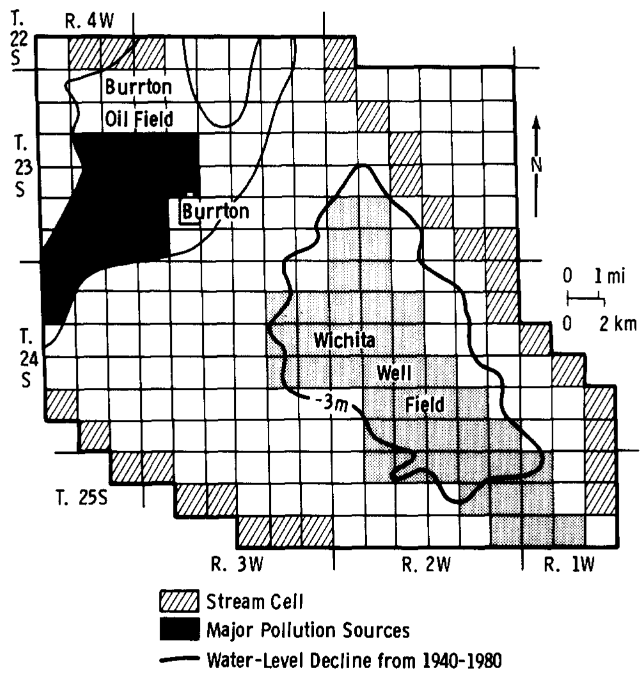

Fig. 8. Location of major pollution sources and extent of the 1940—1980 3-m water-level areal decline.

each section of the indicated area numerous such ponds existed. Such disposal or so-called "evaporation" ponds commonly have an area of 45—930 m^2 and a depth of 0.3—4.6 m. In most parts of the area where such ponds were used, most of the brine escaped by seepage into the previous sandy soils and thence into the aquifer or the streams or both (Williams and Lohman, 1949). According to Williams and Lohman (1949, p. 173),

> "the intrusion of salt water from 'evaporation' ponds into groundwater reservoirs has been proven in many places by analyzing samples of water from nearby wells or test holes, and by experiments indicating that the rate of disappearance of the water is several times as great as it should be based on an approximate average rate of evaporation for Kansas."

Such practices, while inadequately regulated by state agencies during the 1930's and 1940's, were completely outlawed by 1957 (Latta, 1963). The life of operation of each of those ponds is practically unknown, although a figure of ~10 yr. seems to be the right order of magnitude (R. O'Connor, pers. commun., 1982). Brine pollution from other sources such as improperly plugged old holes, natural salt dissolution and other sources constitutes a complex problem. In this study we assume that all brine pollution is lumped into the disposal ponds. The chloride concentration of brines produced from the Burrton oil field (Schoewe, 1943; Rall and Wright, 1953) averages around 10^5 mg l^{-1}. Given the sandy nature of the surficial deposits in the Burrton area and the very shallow water-level depths in the area, we believe that this chloride concentration entered the groundwater system very quickly and was not significantly attenuated.

Despite the previously mentioned data deficiencies, we proceeded with a preliminary chloride-transport modeling effort believing that if we could reproduce the presently observed pattern of chloride concentration, we could have a fairly satisfactory tool for predicting the spatial and temporal chloride patterns, as well as average concentrations in different areas of the aquifer; and that through sensitivity analysis we would be able to evaluate the effect of the various unknown parameters. Although the results of the groundwater-flow model may have been adequate as a first-hand approximation for the general direction and travel time of the chloride solutes, as was mentioned before, the disposal-pond seepage of varied intensity and lifetime, significantly complicates mass-transport predictions. This fact, coupled with the strong desires of the local management district to know in relative detail the spatial and temporal saline-water variations in the area, necessitated this mass-transport modeling approach.

Therefore, using the calibrated steady-state flow model parameters mentioned previously, the detailed 1940 chloride distribution map of the Equus Beds aquifer by Williams and Lohman (1949) as the initial condition (Fig. 9), and the locations of surface disposal ponds (Fig. 8) as the sources of contamination, we used a widely known method of characteristics-solute transport model (Konikow and Bredehoeft, 1978), suitably modified, in our attempts to simulate the water-quality degradation problems of the

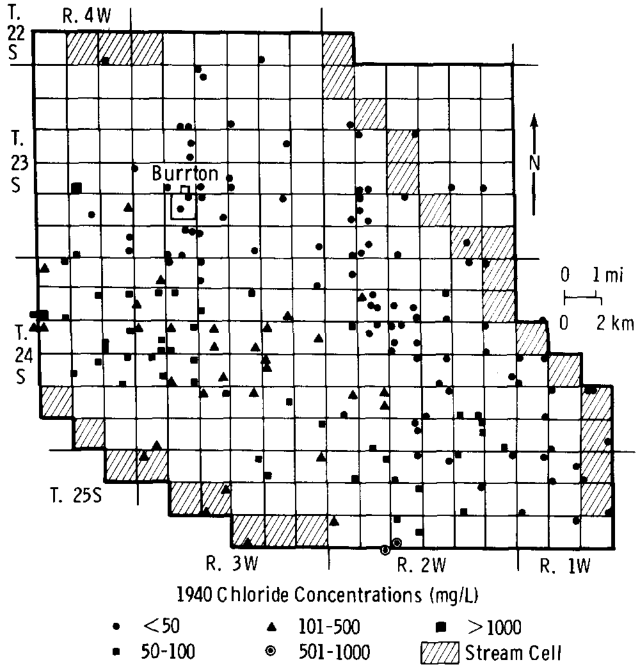

Fig. 9. 1940 chloride concentration of groundwater in the study area.

area. The reader is referred to that publication for details as to the specific form of equations and numerical solution employed. Because the chloride concentrations observed in the aquifer (Fig. 9) are relatively not very high, a constant-density fluid could be assumed. Dirichlet boundary conditions for concentration are prescribed around the perimeter of the study area based on observed data. Generally high chloride concentrations ranging from 200 to 500 $mg\,l^{-1}$ were assigned to the western boundary and along the Arkansas River, while relatively low chloride concentrations (20 $mg\,l^{-1}$) were assigned to the eastern boundary and along the Little Arkansas River. In this study, precipitation-based recharge to the aquifer was assumed to have a chloride concentration of 10 $mg\,l^{-1}$. Various water-quality data were collected over the years, but because of the problems mentioned previously with regard to the quality of these records, we used only recent (1980) water-quality data as benchmark data for comparing observed and simulated chloride distributions. Sensitivity analysis, the results of which will be presented in the next section, proved to be instructive in selecting mass-transport parameters.

Recently Sophocleous (1982) has comparatively evaluated the performance of three different mass-transport modeling methodologies as typified by three, widely known, finite-difference, method of characteristics, and finite-element models, by applying them, under identical conditions, to the actual Equus Beds aquifer study area. A simultaneous comparison of all three simulated chloride distributions with the observed values indicated that the method of characteristics approach most frequently matched the observed data in this particular case study, followed closely by the finite-element method. Such results indicate that in cases where the convective term of the mass-transport equation predominates over the dispersive term, as is the case here, the method of characteristics approach seems a better approach to follow as compared to the finite-difference or finite-element approaches considered in Sophocleous (1982).

SENSITIVITY ANALYSIS AND RESULTS

Numerous computer runs were executed to check the sensitivity of the adopted MOC model to various solute transport parameters and pollutant sources. The model is shown to be very sensitive to the effective porosity (ϕ) value used, relatively sensitive to the longitudinal dispersivity (α_L) value, but not very sensitive to the ratio of transverse to longitudinal dispersivity (α_T/α_L). The relative insensitivity of the model to dispersivity adjustments is probably caused by the large grid size of the model. However, it could be seen (Fig. 10) that, as the value of dispersivity and porosity increased, the chloride solute moved farther through the flow system and the concentration gradient decreased. Several values of porosity, longitudinal dispersivity, and ratio of transverse to longitudinal dispersivity were employed and the chloride distribution was computed after 40 yr. of simulation. Some of the results are shown in Fig. 10 for the $> 1000\text{-mg-l}^{-1}$ chloride concentration. More than 45 laboratory porosity determinations from several areas of the Equus Beds aquifer (Williams and Lohman, 1949) indicated that the average value of effective porosity of 0.30 employed in this model is of approximately the right value. A study of the chloride distribution, both during the present and during the early 1940's, shows high chloride concentration contrasts in nearby locations, indicating relatively low dispersivity values. The value of 30 m for the longitudinal dispersivity produced a satisfactory match between observed and calculated chloride distributions, although the confidence on this dispersivity value may not be very high because of the large spatial grid used in this study. However, the fact that in this field application the convective term predominates over the dispersive term in the mass-transport equation, and that field observations, as previously mentioned, suggest a small value of dispersivity indicates that this issue is non-critical.

It was also found that the simulated chloride distribution was very sensitive to the brine concentration entering the groundwater system as well as to the rate of disposal-pond seepage. Fig. 11 shows the results of doubling the rate of seepage or the concentration in the percolating water. Of course,

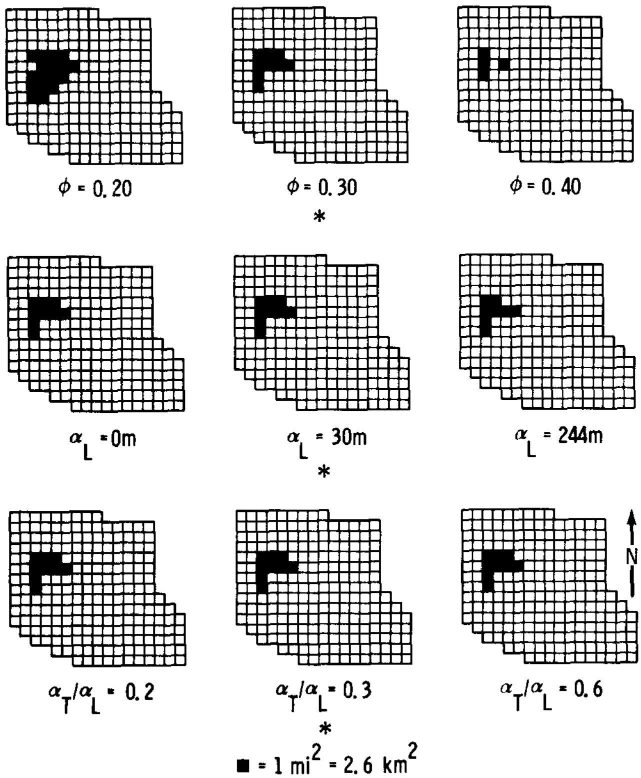

Fig. 10. Model sensitivity to various parameters as indicated by the $> 1000\text{-mg-l}^{-1}$ chloride distribution after 40 yr. of simulation. An *asterisk* indicates the adopted parameter value.

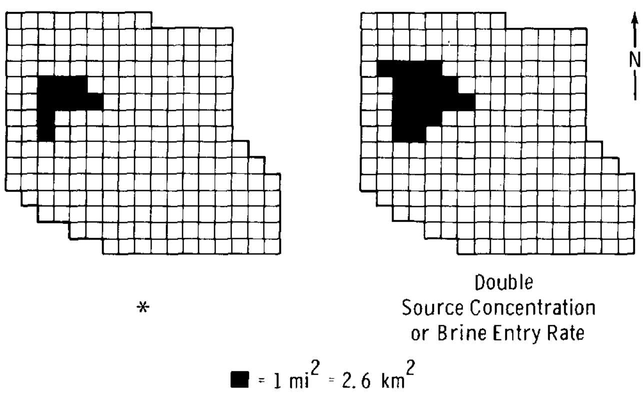

Fig. 11. Effects of doubling the rate of seepage or the concentration of the percolating oil-field brine on the $> 1000\text{-mg-l}^{-1}$ chloride distribution after 40 yr. of simulation.

the initial concentration distribution, as well as the location of disposal ponds, is very important.

Given the above results, and having obtained a calibrated groundwater-flow model, an effective way to reproduce the present chloride concentration is to manipulate the sources of pollution by adjusting, within limits, both the concentration of the brine entering the aquifer and the rate of brine percolation rate. A comparison of measured and simulated results is shown in Fig. 12. The match between observed and calculated results seems to be satisfactory, given that the model predicts average concentrations over a 2.6-km^2 area. Once a match to the historical data was obtained, chloride concentration projections for the year 2000, as indicated by the >1000-mg-l^{-1} chloride distribution, were made (Fig. 13). This projection shows that the brine plume, in a relatively diluted form, would barely reach up to within 1.6 km of the westernmost edge of the Wichita well field by the year 2000, provided that the drawdown in the Wichita well field does not increase

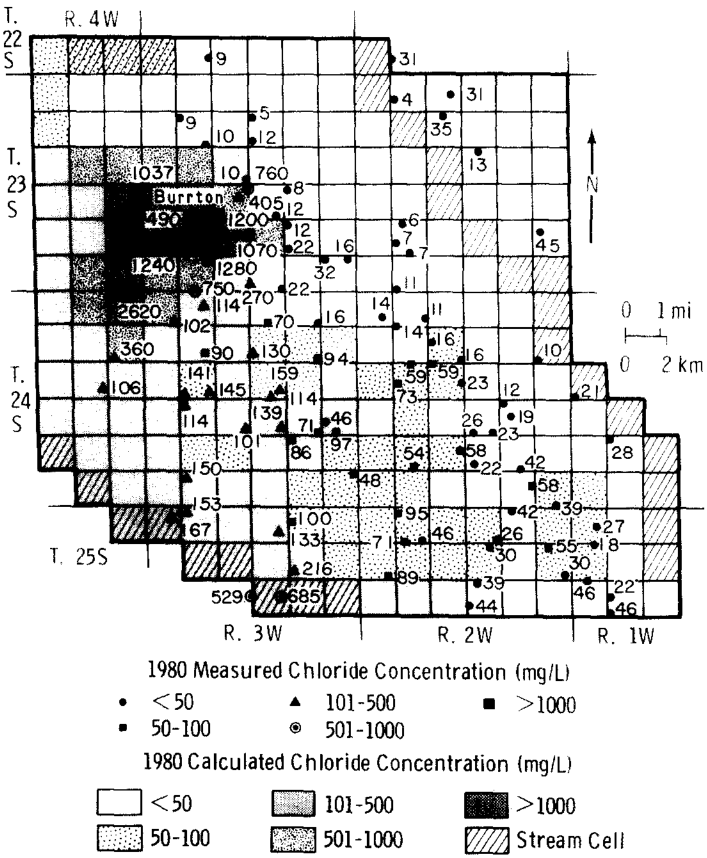

Fig. 12. Comparison of measured and simulated chloride concentrations.

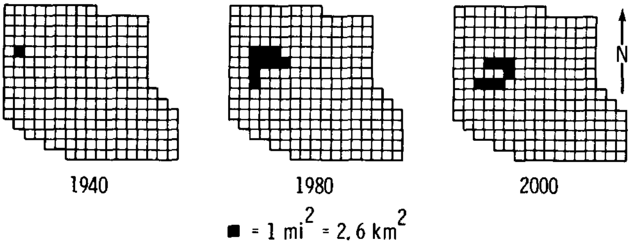

Fig. 13. Historic evolution and future projection of the $>1000\text{-mg·l}^{-1}$ chloride concentration.

significantly during the prediction period. Because the cone of depression caused by the Wichita well-field pumpage, as indicated by the 3-m 1940—1980 water-level decline contour (Fig. 8), has not yet been extended significantly beyond the boundaries of the well field, we believe that the results of the present simulation are valid. However, if drawdown increases in the Wichita well field, then the brine may be drawn into it much more quickly.

A FREQUENT DILEMMA

Given the uncertainties with regard to pollution-source concentrations and rates, among other questionable parameters in a mass-transport modeling study such as this one, one could justifiably wonder if it is worthwhile at all to tackle the complexities of an inverse or parameter estimation problem in order to get a better handle on the groundwater flow field. In an attempt to answer this question, we ran a number of simulations to see what effect groundwater-flow parameters different from the best estimates (Table I), derived through the flow calibration, would have on the present simulated chloride concentration distribution starting from the 1940 initial conditions. The dilution effects of increased recharge, and the brine-plume transmission downgradient in the flow field when transmissivity was increased were evident from such simulations. The differences in concentration resulting from using the best estimates of flow parameters (Table I) vs. the prior estimates (Table II), as indicated by the $>1000\text{-mg·l}^{-1}$ chloride concentrations (Fig. 14), were significant enough to justify a parameter estimation effort.

This result supported our educated guess that, in each modeling phase in a study, one does the best possible job in calibrating the model, thus reducing to a degree the uncertainty in that phase, hoping that when improved estimation procedures are developed, they could be directly applied to the calibrated model. Unfortunately, however, in many instances, like this one, where the pollution problem appeared 30 or 40 yr. after the actual pollution sources had been emplaced and since disappeared, it seems that

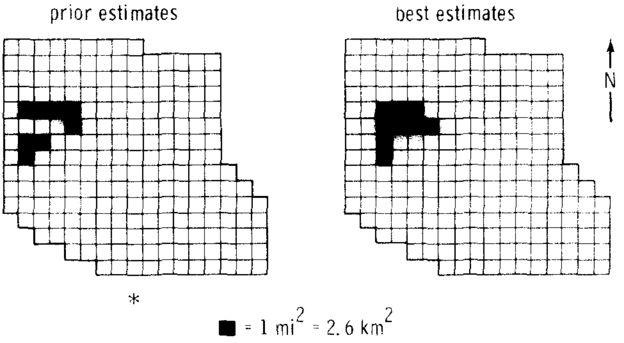

Fig. 14. Effects of using the prior or initial estimates (Table II) vs. the best flow parameter estimates (Table I) on the chloride concentration distribution as indicated by the > 1000-mg-l^{-1} chloride concentrations after 40 yr. of simulation.

there is not much one could do to estimate the historic pollution-source concentrations and rates, if no detailed records are kept. Nevertheless, usually there are some reasonable estimates that could be adjusted within limits. The parameter estimation procedures for mass-transport models are further behind the state of groundwater-flow parameter estimation procedures, which are still at their initial stages. An emphasis on these aspects is urgently needed.

GENERAL CONCLUSIONS

(1) The multiple-regression procedure for estimating the parameters contained in groundwater models and the statistical techniques for analyzing the models are useful and powerful tools for applying groundwater models to real field problems. In this study, the regression modeling approach gave a more accurate velocity field for transport modeling than a model based on the available parameters.

(2) Many input data are required for the groundwater flow and mass-transport models and the reliability of the modeling results is affected by the accuracy of these data. A sensitivity analysis helps in the definition of accuracy requirements for each of the input parameters.

(3) The models employed in this study performed satisfactorily despite data deficiencies and modeling errors. Although the present solute-transport model should be regarded only as a "first-approximation" attempt, the overall water-quality patterns of the observed and calculated data are in fairly good agreement. Changes in the chloride concentration of the groundwater were predominantly controlled by past oil-field brine disposal practices, convective transport, and mixing and dilution with recharge water of low chloride concentration.

(4) The water-quality modeling results indicate that the chloride concentration of the Wichita well-field waters will not have deteriorated from their present condition by the year 2000, provided that the drawdown in the Wichita well field does not increase significantly. However, the brine plume is shown to be moving southeastwards in a relatively diluted form (Fig. 13), but still rendering the chloride concentration of groundwaters in that general direction above the recommended drinking limits. Therefore, it would be prudent to continue saltwater monitoring efforts.

(5) The predictive capability of the model can be helpful in expanding the present saltwater monitoring network. By indicating the most probable and least probable areas of future contamination and the rate of spreading, optimal locations and sampling frequencies for observation wells can be determined. It may also be both physically and economically feasible to institute a reclamation program to improve or control the quality of groundwater. An accurate model of flow and solute transport in the aquifer could be an invaluable tool for planning an efficient and effective water-management plan.

ACKNOWLEDGMENTS

Faisal Latif in his capacity as student research assistant ably assisted in the various aspects of computer implementation of the numerical models. Leslie Smith of the University of Vancouver made a number of useful comments in reviewing an earlier version of this paper. This work was supported in part by the Office of Water Research and Technology of the Bureau of Reclamation, U.S. Department of the Interior.

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