WATER QUALITY MODELING OF THE EQUUS BEDS AQUIFER IN SOUTH-CENTRAL KANSAS

by

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ABSTRACT

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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 hyraulic head. A chloride transport modeling effort is then carried out despite some serious data deficiencies, the significance of which are evaluated through sensitivity analysis. Three mass-transport models employing a finite difference, a finite element and a method of characteristics approach are comparatively evaluated by applying them to the study area. It is concluded that in cases where the convection term predominates, as is the case with the study area, the method of characteristics is the better procedure to follow. 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.

ACKNOWLEDGMENTS

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Kaye Long, Secretary for the Geohydrology Section of the Kansas Geological Survey, typed the manuscript. The Kansas Geological Survey's Graphic Arts Section prepared most of the figures.

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INTRODUCTION

The Equus Beds aquifer in south-central Kansas plays a vital role in the economic well being of the municipal, industrial and agricultural communities in that area of Kansas. The continuously increasing demand for groundwater together with industrial and municipal activities generate or facilitate pollutants which threaten the quality of groundwater. Therefore, steps must be taken to protect the quality of groundwater subject to the demands and requirements of the area. This study represents one such step.

OBJECTIVES

The three main objectives of this project are:

1. To evaluate several existing numerical mass transport models designed to predict groundwater degradation due to contamination of aquifers by natural and/or man-made pollutants.

2. To modify and adopt one or a combination of these models that would produce the most reliable results with reasonable amounts of computer time and storage.

3. To apply this model to a critical part of the Equus Beds aquifer, including a calibration of the groundwater flow model and, depending on the adequacy of available data, of the mass transport model also.

All the three above-mentioned objectives have been met. Another objective, originally planned, relating to an application of a management model to minimize the rate of salt water intrusion in the same area, while satisfying the demand constraints is currently near completion as a separate Kansas Geological Survey study.

STATEMENT OF THE PROBLEM

In recent years it has become clear that the groundwater quality in parts of the Equus Beds aquifer (Fig. 1), which is of great importance for south-central Kansas and the City of Wichita, 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 about three 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 1930s and 40s (Williams and Lohman, 1949; Latta, 1963; Leonard and Kleinschmidt, 1976). Locally, pollution by saline water has also 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 disposal 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 fresh-water 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. 2), 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

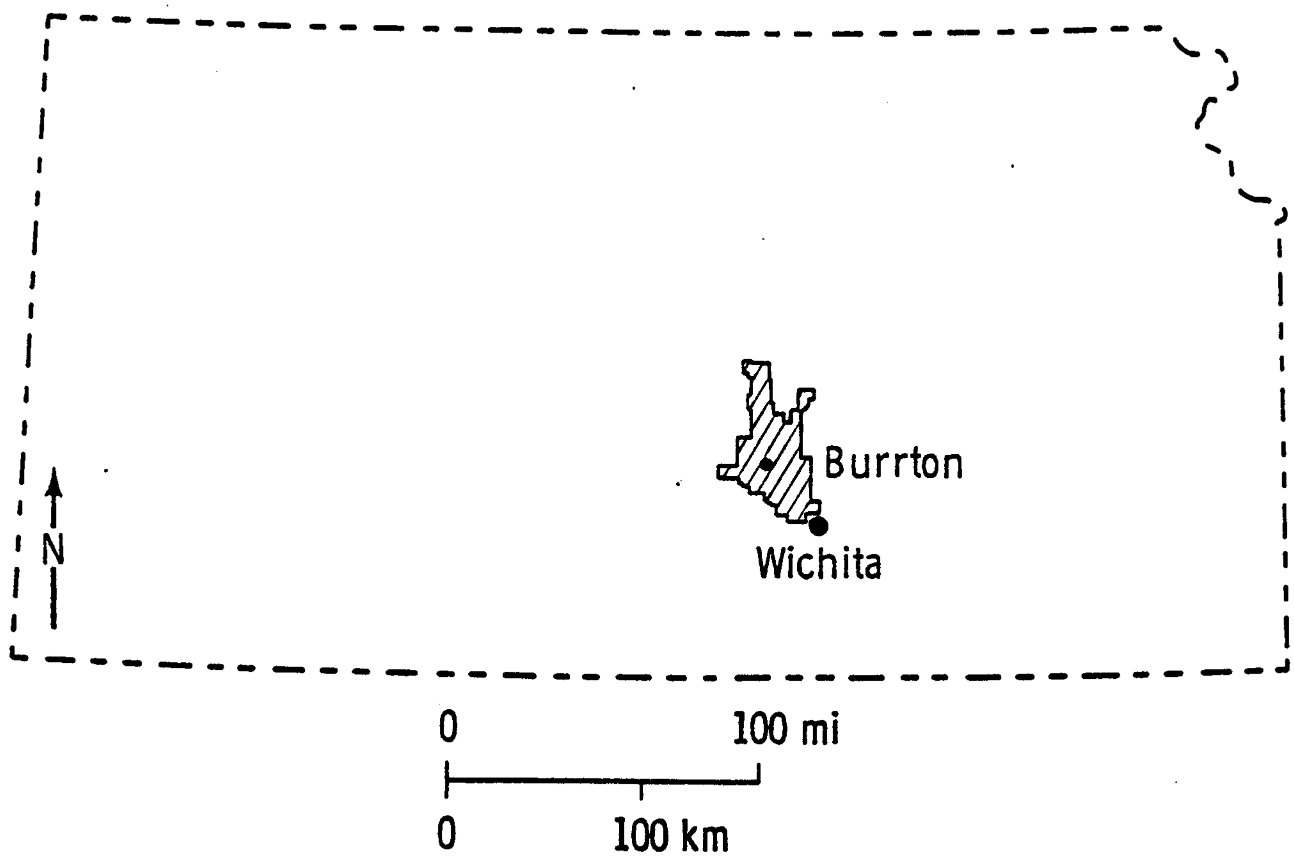

Figure 1. Location map within Kansas.

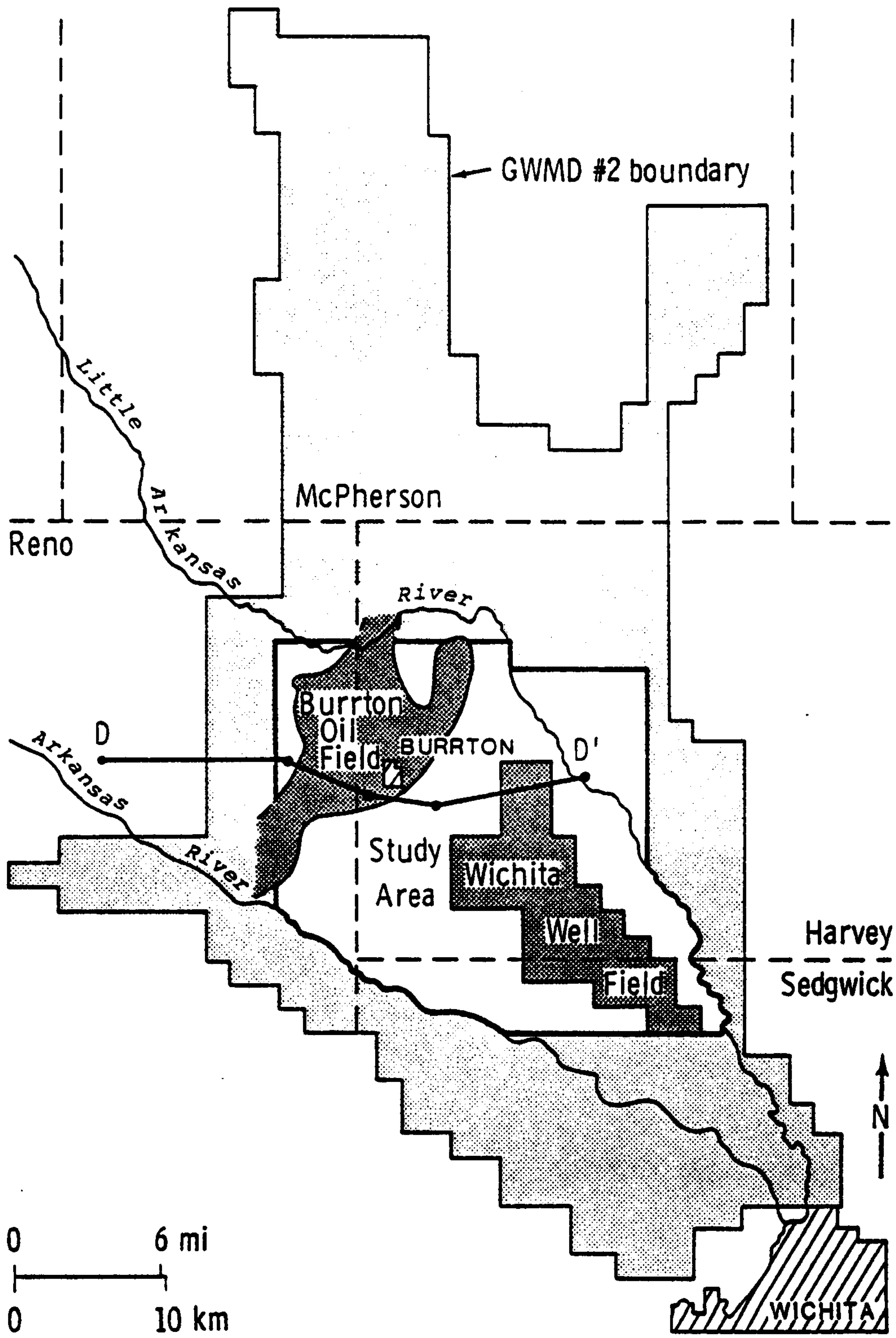

Figure 2. Equus Beds aquifer as indicated by the boundaries of the Equus Beds Groundwater Management District, and study area.

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. 3) and are in the proximity of oil fields, both sources of brine.

Groundwaters from the Equus Beds aquifer normally contain less than 100 mg/l 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. Nevertheless, sodium to chloride ratios (Na/Cl) can be used to differentiate between the two sources of brine pollution (Leonard and Kleinschmidt, 1972; Hathaway, et al., 1981; Whittemore, et al., 1981). Na/Cl ratios of brines from the lost-circulation zone are generally higher than 0.6, while oil-field brines from the Equus Beds area average about 0.5. Application of these ratios to the determination of the type of brine pollution is not always straightforward, because cation-exchange reactions within the aquifer may modify the initial ratios observed in the original brine solutions. A detailed study of the variations in concentration of selected trace constituents such as bromide, iodide, boron, and lithium relative to that of a conservative major component such as chloride are proven useful in more definitive determination of pollution sources in the area (Whittemore, et al., 1981).

Geochemical evidence based primarily on Br/Cl ratios (Fig. 4) 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; Whittemore and Basel, 1982). The curves indicated on that figure represent the boundaries of mixing zones of freshwaters with oil-field brines and halite solutions (Whittemore and Basel, 1982). Most of the groundwater samples from the Equus Beds monitoring wells with chloride concentrations above 250 mg/l fall within the freshwater/oil-field-brine mixing zone (Fig. 4). In general, the concentration of chloride increases with depth in the aquifer. The relation could be caused by upward movement of saline water through fractures in the bedrock or through wells. However, this stratification is probably caused by the infiltration of dilutant rainfall and

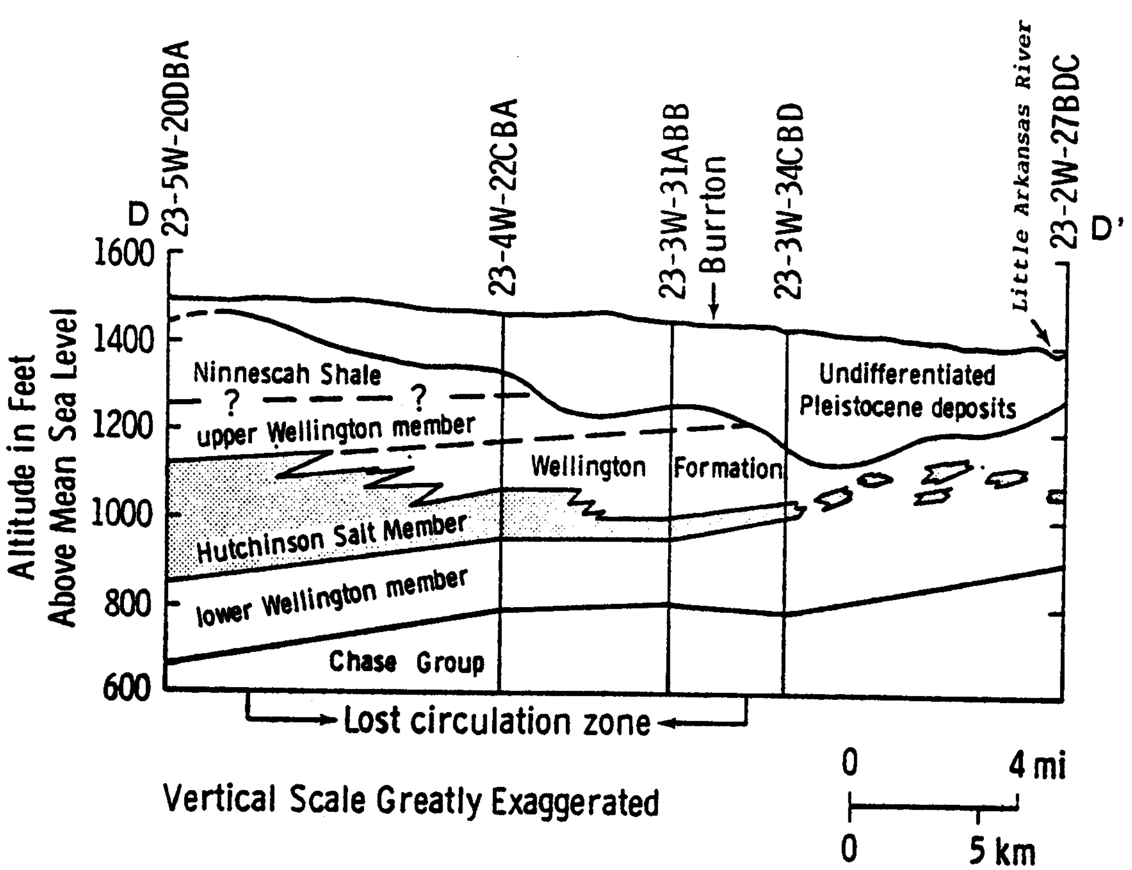

Figure 3. Geologic cross section in the vicinity of Burrton. To convert values in feet to values in meters, multiply by 0.305.

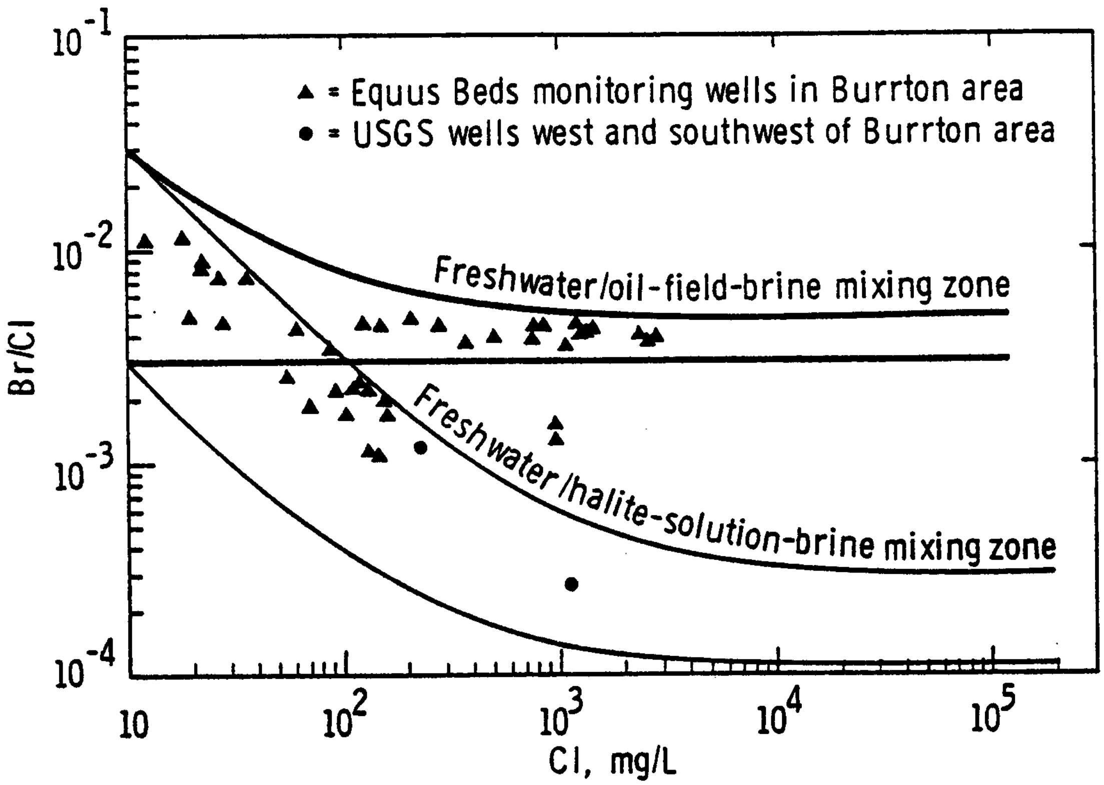

Figure 4. Identification of saltwater sources in the Burrton Area.

the fact that saline water is denser than fresh water (Leonard and Kleinschmidt, 1976). In the vicinity of disposal ponds, the highest concentration of chloride normally occurred near the surface (Williams and Lohman, 1949). I/Cl ratios also suggest that saltwater originated at or near the surface (Whittemore and Basel, 1982) and flowed downwards through the freshwater aquifer. This is because, unlike bromide, iodide in saline waters can be adsorbed by clays in the sediments. Therefore, as brine is dispersed through the fresh-water aquifer, the I/Cl ratios may decrease relative to those of Br/Cl, as was actually observed in comparing shallow and deeper waters in the aquifer (Whittemore and Basel, 1982). Because of the nonhomogeneity of the aquifer deposits, higher concentrations of saline water can occur anywhere in the saturated section.

In the area adjacent to the western part of the Wichita well field relatively high concentrations of chloride are increasing with time as a result of lateral migration of saline water from the vicinity of the Burrton oil field and from the Arkansas River Valley (Fig. 5). For those reasons, local authorities are very concerned about the temporal and spatial expansion of this brine plume. However, in the areas of greatest drawdown in the Wichita well field, the maximum concentration of chloride has not increased appreciably since the 40s, while in some parts of the well field the chloride concentrations have decreased slightly (Leonard and Kleinschmidt, 1976). A study of the groundwater velocities in the area, which are in the eastern to southeastern direction, reveals that groundwater velocities in the Equus Beds aquifer outside the well field area average about 0.3 m/day, while in the well field area they average about 0.6 m/day (Sophocleous, 1982; Stramel, 1956). Assuming that the so-called "Burrton brine plume" originated one mile west of Burrton and that dispersion-diffusion effects are negligible, it would take about 80 years for that plume to be convected by the southeasterly moving groundwater to reach the westernmost edge of the Wichita well field. Also, assuming that the Burrton brine plume originated during the late 30s, it would have by now passed the half-way mark of that distance, a phenomenon actually observed today.

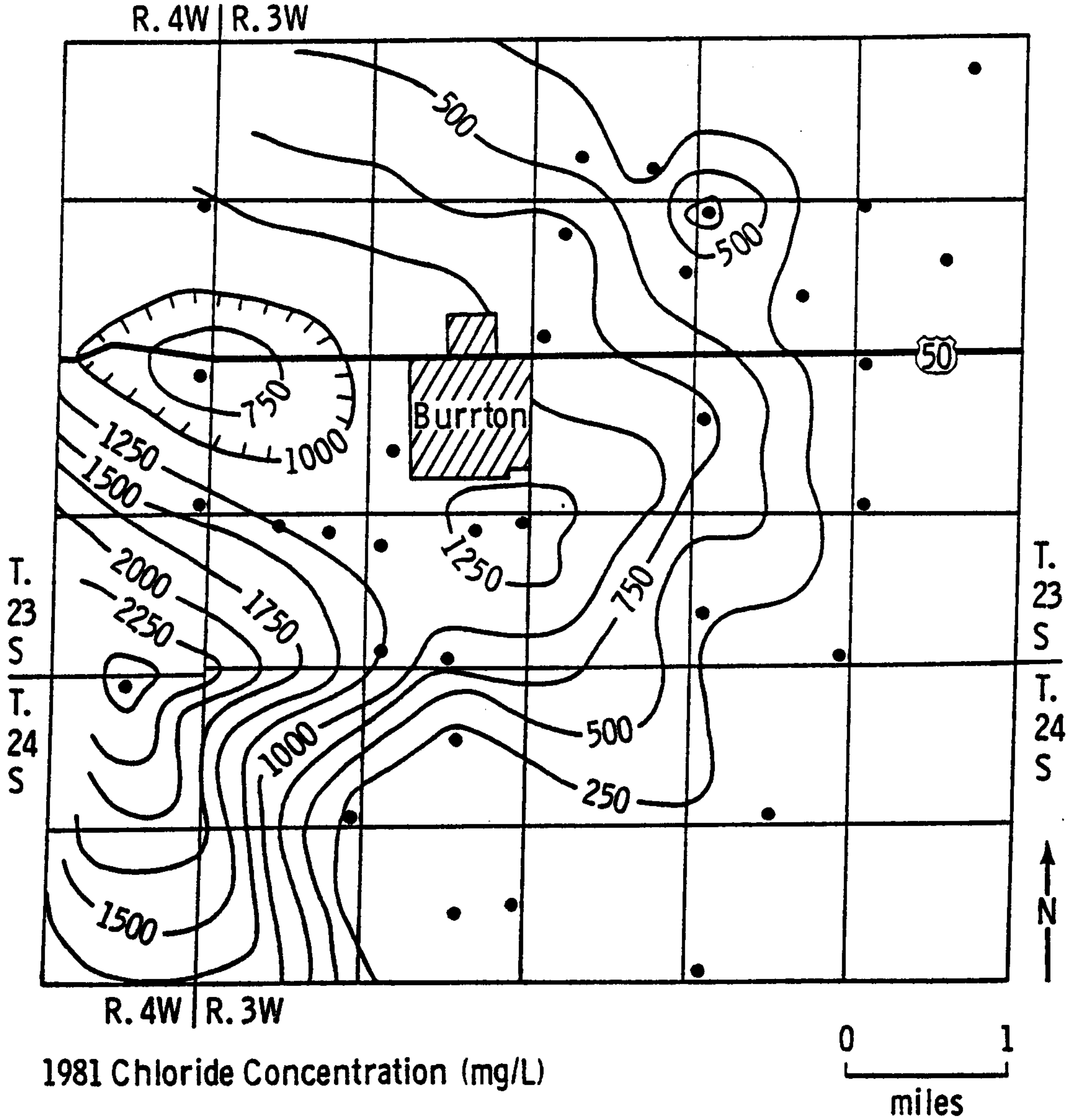

Figure 5. 1981 chloride distribution for the Burrton area.

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 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 development, 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 240 square-mile area in the vicinity of Burrton, where most of the suspected groundwater pollution is taking place or took place in the past (Fig. 2) 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 40s. 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. 6). 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

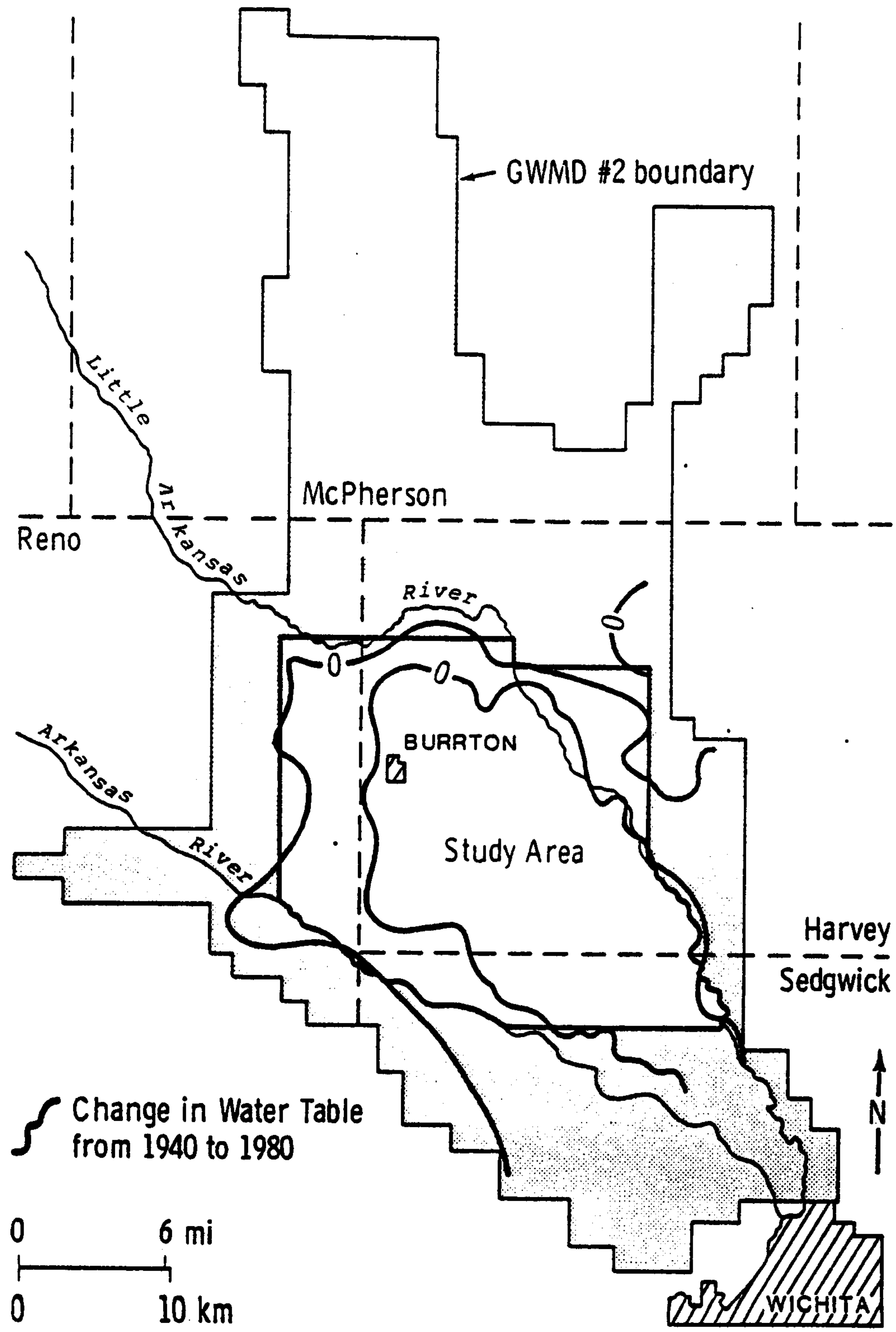

Figure 6. 1940-1980 zero water-level decline contours for the study area.

conditions along the boundaries of the area. The Arkansas River, the largest stream, is used as a constant head boundary in the southwestern boundary of the study area, while the Little Arkansas River is considered as a constant head boundary at the southeastern boundary of 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 40s 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. 3), which is the predominant bedrock unit in the study area, can be divided (Leonard and Kleinschmidt, 1976) 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. 7). The Equus Beds aquifer is recharged principally from precipitation, which averages about 76 cm per year. 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 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 measured in the field or laboratory, or estimated 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 behavior, 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

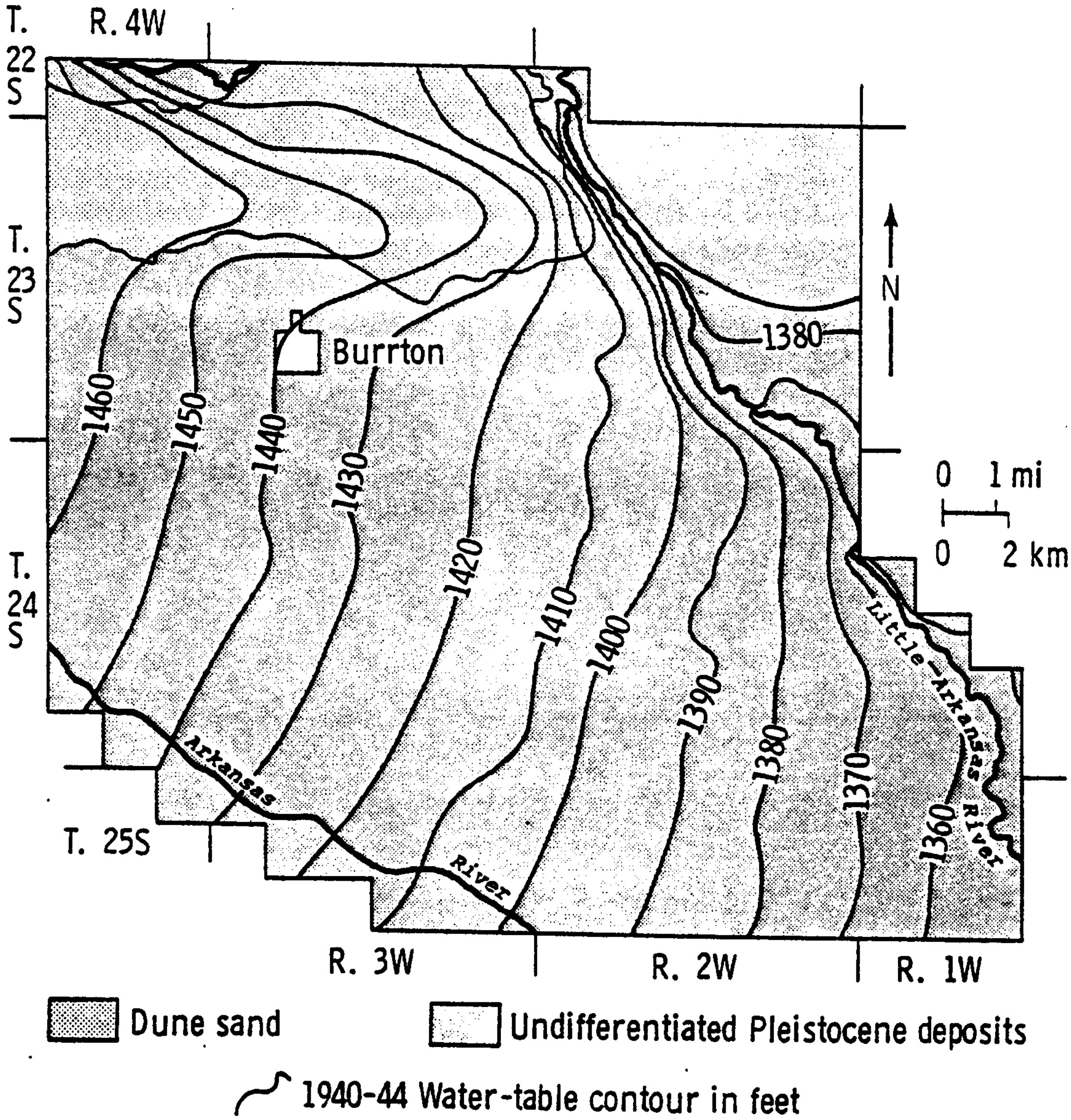

Figure 7. Surficial geology and 1940-44 water-table configuration.

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 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:

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

where for areal flow

T_{ij} is the transmissivity tensor $[L^2T^{-1}]$;

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) $[LT^{-1}]$; 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 eqn (1) with its attendant boundary conditions cannot be solved analytically. Thus, the regression solution must be based on a numerical solution of (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 eqn (1) 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

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

where $\underline{h}^{obs}$ is the vector of observed heads, $\underline{h}$ is a vector of predicted heads, $\underline{e} = h^{obs} - h$ 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 that describes the reliability of h^{obs} at each node. If for observation ℓ, $w_\ell = 0$, 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 (3) with respect to each parameter may be written as

$$\underline{e}^T\,\underline{w}\,\frac{\partial \underline{e}}{\partial \underline{b}} = 0 \tag{4}$$

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 (2). The technique yields a regression equation, which upon convergence of the procedure may be written as

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

where $\underline{X}^n$ 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 (2) for $\underline{h}$, which is the subset of $\underline{h}_m$ applying at nodes that are observation nodes, can be written for observation ℓ as

$$h_\ell^{obs} = f(\xi_\ell, \beta) + \varepsilon_\ell \tag{6}$$

where f indicates a function that is the solution of (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.

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

$$E(\varepsilon_\ell) = 0 \tag{7}$$

$$Var(\varepsilon_\ell) = \sigma^2 \tag{8}$$

$$\mathrm{Cov}(\varepsilon_\ell, \varepsilon_m) = 0 \qquad \ell \neq m \tag{9}$$

where E, Var and Cov are the expected value, variance and covariance operators. 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 ($\ell \neq m$) 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 Figure 8. 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 (1 mi^2) blocks or were located very near to them (generally less than 0.4 km (0.25 mi) from the 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 large grid 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 Figure 8, 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 zonation is

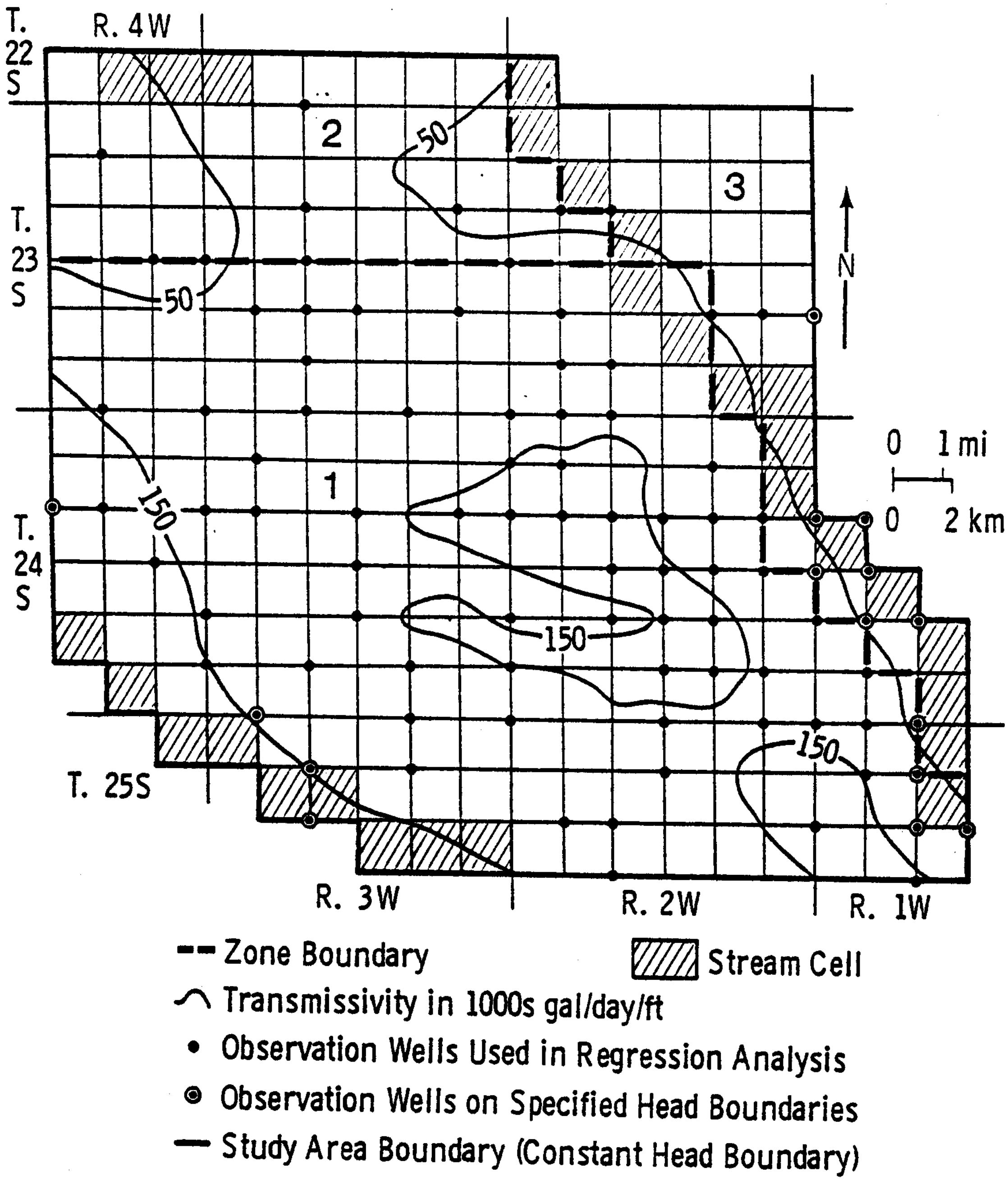

Figure 8. Location of observation wells and hydrogeologic zonation in the study area. To convert transmissivity contours in 1000s gal/day/ft to m^2/day, multiply by 12.42.

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 also. 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. 8), while recharge is allowed to differ. Transmissivity for zone 1 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. 8), while recharge for zone 2 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. The values of specified hydraulic head along the boundaries were estimated from the 1940-44 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 1. 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 less than the model response as indicated by the maximum head loss $\Delta h = 44.8$ m.

TABLE 1

Summary of Parameter Estimation Results for the Equus Beds Aquifer

Zone	Transmissivity m^2/day	Std. Error m^2/day	Recharge m/day x 10^{-4}	Std. Error m/day x 10^{-5}	Leakance day^{-1} x 10^{-4}	Std. Error day^{-1} x 10^{-4}
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).

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 ith parameter is given by the square root of the ith diagonal component of the variance-covariance matrix $(\underline{X}^T\underline{wX})^{-1}$ s^2, where s^2 is the sample error variance. Examination of Table 1 indicates that the standard errors for the parameters are generally less than 25 percent of the magnitude of the respective parameters. Comparison of the estimated sum of squared errors or error variance obtained using these parameter estimates (Table 1) to the error variance obtained using the initial estimates (Table 2) shows an error variance reduction of more than 57.2% as a result of the parameter estimation procedure.

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 2). 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, resulting from employing the previously-mentioned multiple regression procedure, can occur. In such cases, the singularity problem can be rectified by using prior information. Also, in cases where the only source of singularity is that a column of the sensitivity matrix $\underline{X}_j=0$, 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.

Figure 9 shows plots of the scaled sensitivities, $\underline{Z}$, of the head distribution with respect to the recharge, transmissivity and leakance

TABLE 2

Prior Estimates of Regression Parameters for the Equus Beds Case Study*

Zone	Transmissivity m^2/day	Recharge m/day x 10^{-4}	Leakance day^{-1} x 10^{-3}
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.

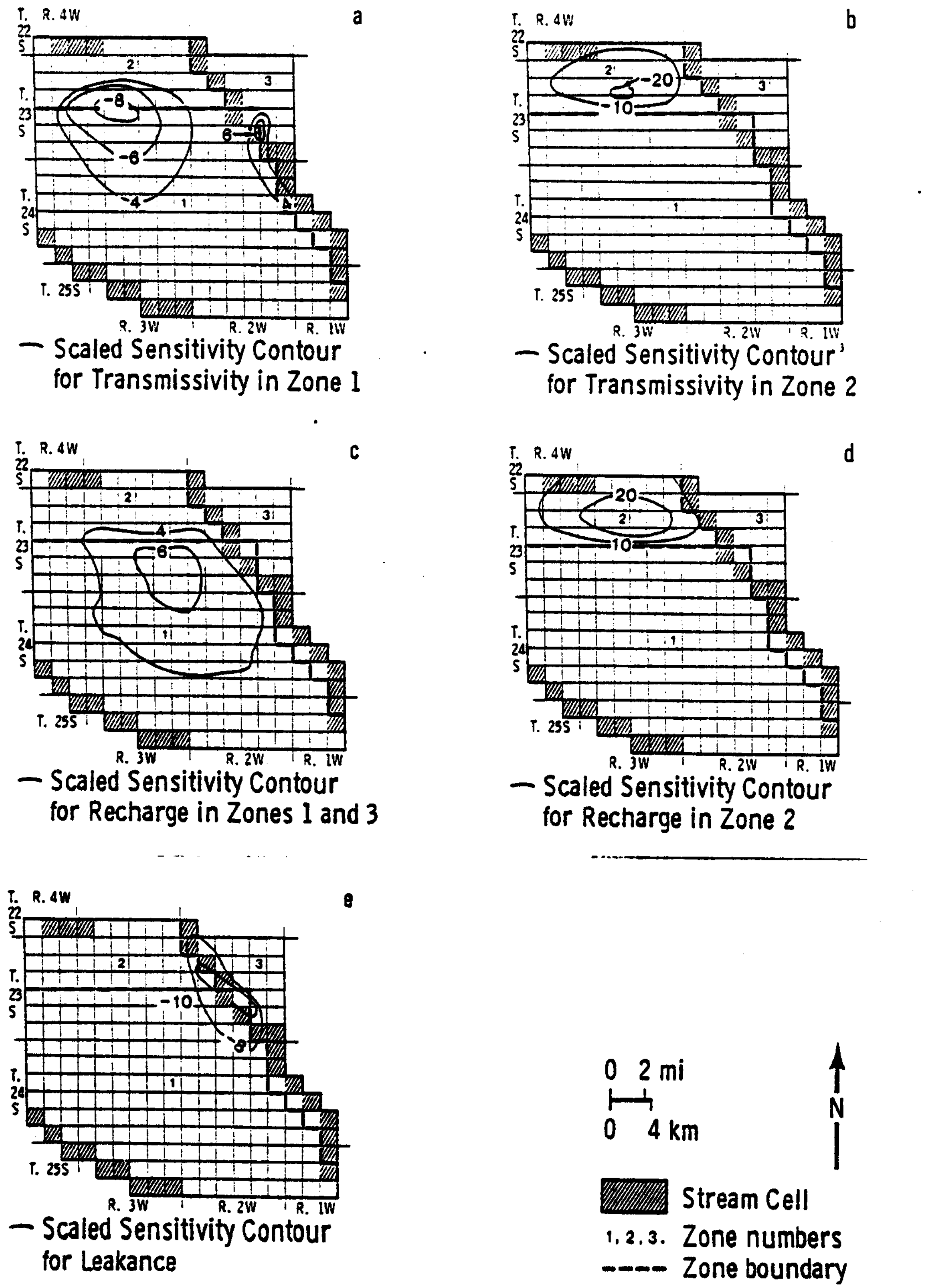

Figure 9. Scaled sensitivity contours for transmissivity (a,b), recharge (c,d), and stream leakance (e).

parameters for all three zones. The scaled sensitivities, $\underline{Z}$, are sensitivities scaled with respect to the parameters, that is $\underline{Z} = \underline{X} \cdot \underline{B}$, where $\underline{B}$ = diag. $(b_1, b_2, \ldots, b_p)$. The computed head distribution is least sensitive to transmissivitiy and recharge for zones 1 and 3 (Fig. 9a, 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. 9d, b), where recharge and hydraulic gradients are both high. The head distribution is also relatively sensitive to the leakance value (Fig. 9e). 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 Figure 9 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. In Figure 10, residuals are plotted against values of estimated head. No relationship of significant concern is visually obvious. The residuals were also plotted against Cartesian coordinates (Fig. 11). The residuals show no obvious systematic variation of significant degree over the map area, indicating that this model is probably adequate for these data.

In order to check if the residuals form a normally distributed sample, they have been plotted on normal probability paper (Fig. 12). A relatively well-fitting straight line is drawn through the bulk of the points plotted,

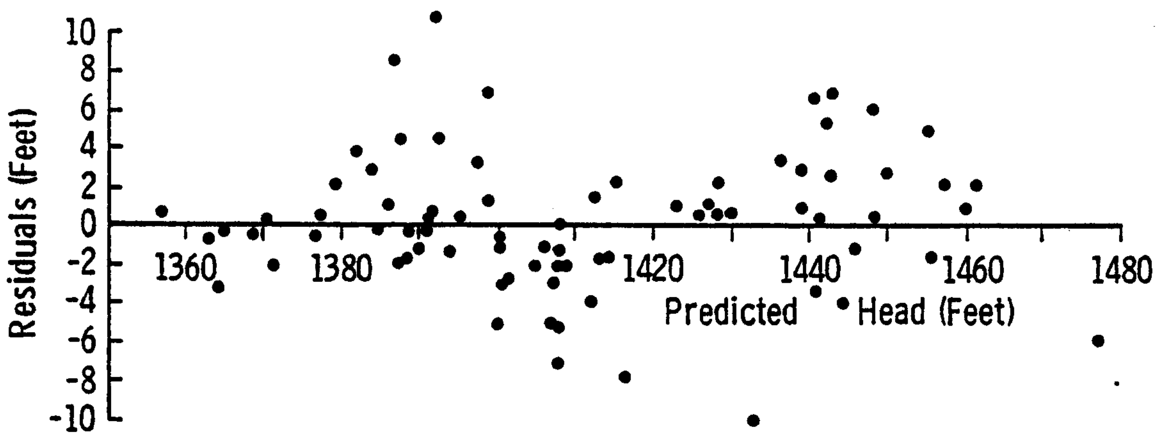

Figure 10. Residuals plotted against calculated head values. To convert values in feet to values in meters, multiply by 0.305.

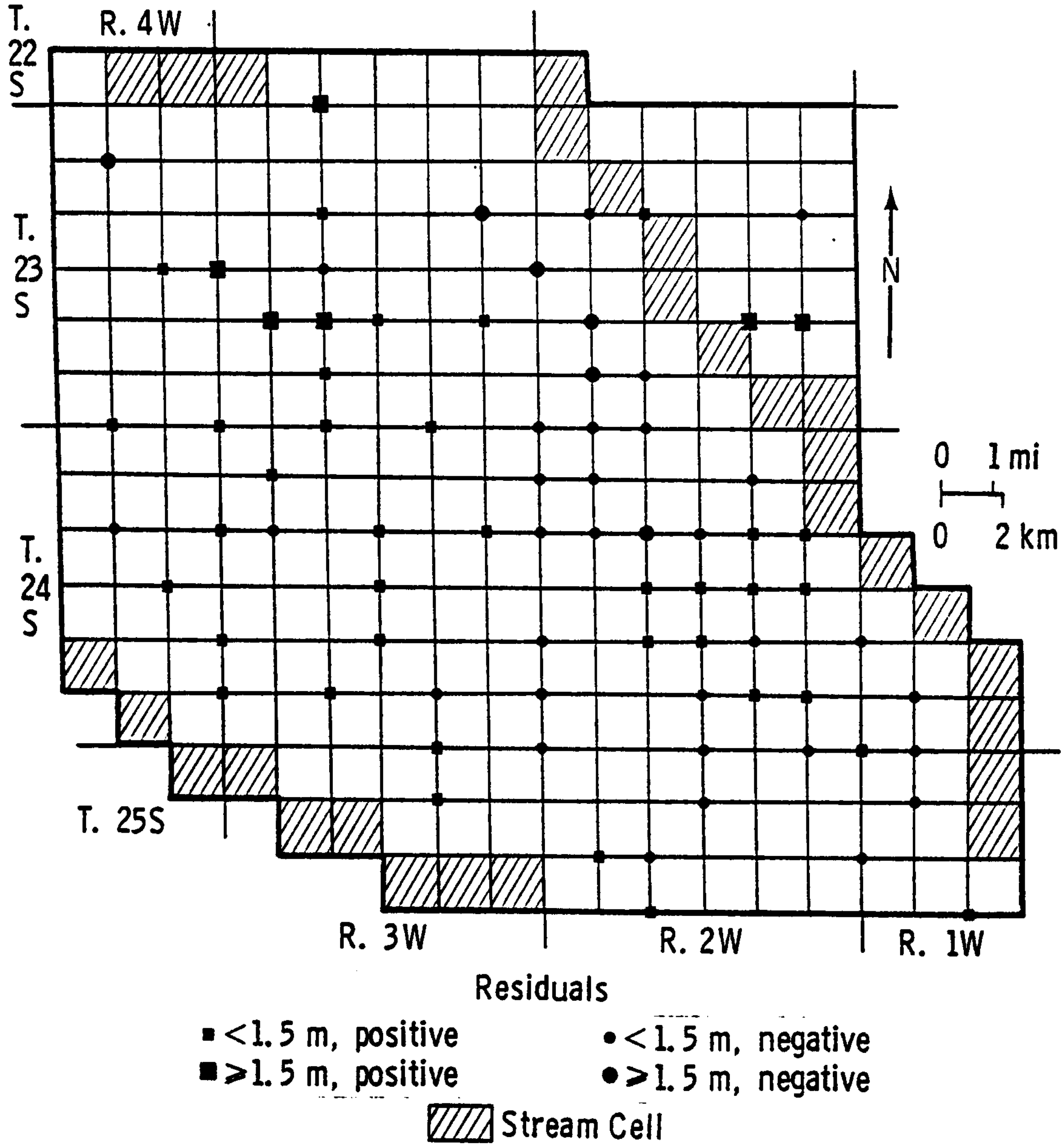

Figure 11. Residuals plotted against Cartesian coordinates.

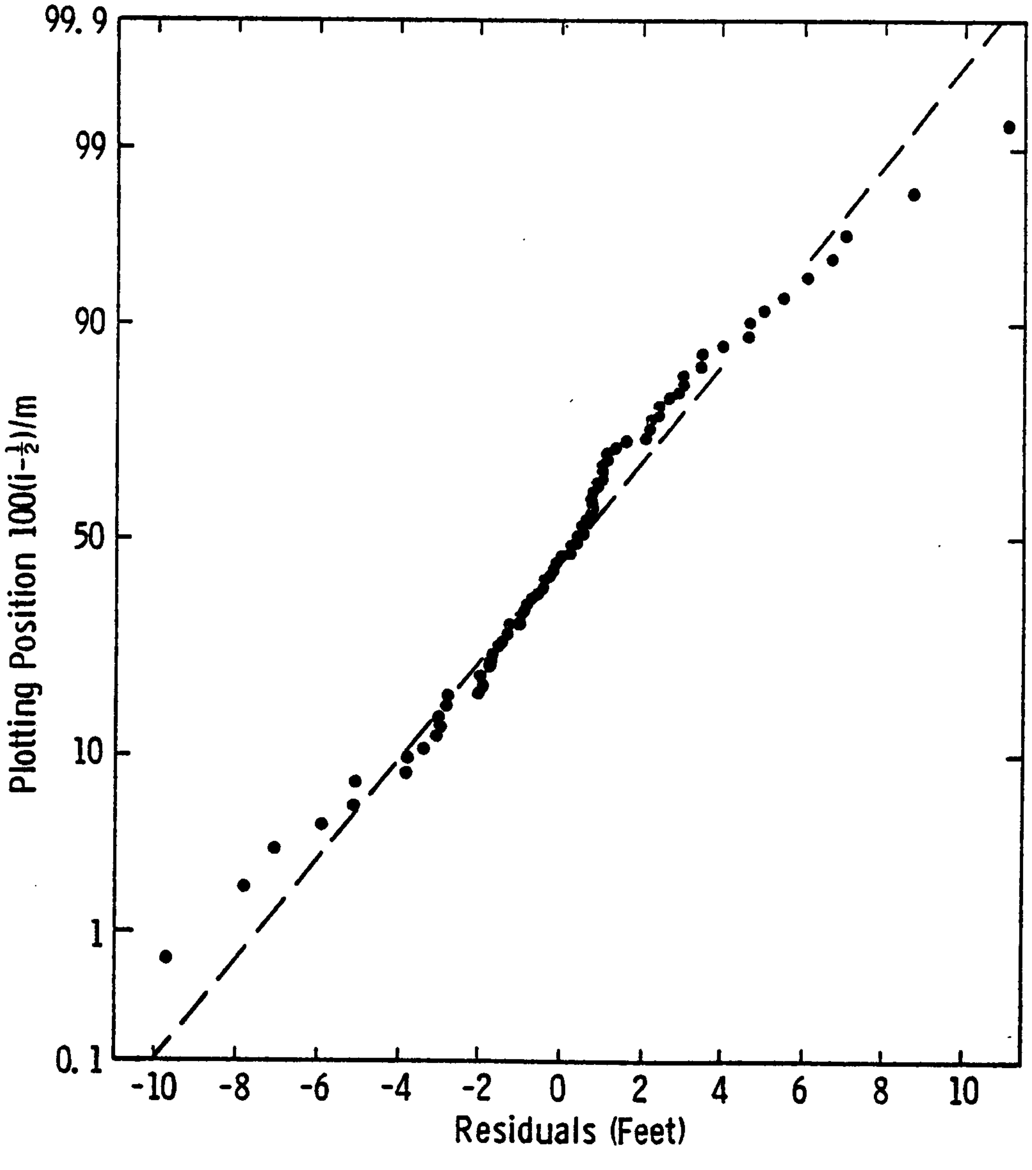

Figure 12. Normal plot of the residuals. To convert values in feet to values in meters, multiply by 0.305.

indicating that the calculated residuals are approximately normally distributed. For the parameters derived by the least squares analysis to be maximum likelihood estimates of the true parameters, residuals must be normally distributed.

MASS TRANSPORT MODELS CONSIDERED

Once the groundwater flow model was obtained and calibrated, the next step was the formulation of a mass transport model. As was mentioned in a progress report on this study (Heidari, et al., 1981), numerous flow and mass transport codes, including also unsaturated-saturated ones and three-dimensional ones were considered for possible adoption in this study. After preliminary check runs of these codes, and after compiling and evaluating the relevant available data that are required in implementing these numerical codes for the Equus Beds aquifer, we decided to restrict ourselves to one code from each of the three already well-established methods of solution of the solute transport equation, namely the finite difference (FD), the method of characteristics (MOC), and the finite element (FE) approaches. Because of lack of adequate and/or reliable data, we decided to eliminate three-dimensional, unsaturated-saturated, stratified cross sectional, and multispecies and reactive solute transport models, and restrict ourselves to two-dimensional, areal, saturated, and non-reactive species-type models. Because the chloride concentrations observed in the aquifer are not sufficiently high, a constant density fluid could be assumed. The models we decided to consider for this study are: Konikow's and Bredehoeft's (1978) MOC model, which is also the standard USGS mass-transport code, Grove's (1977) FD model, and Pinder's (1979) FE model, known as ISOQUAD4.

All those models are programmed to solve the two-dimensional form of the following mass-transport equation:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(Cv_i) - \frac{c'W^*}{\phi} + \sum_{k=1}^{s} R_k \qquad (10)$$

where $v_i = -\frac{K_{ij}}{\phi}\frac{\partial h}{\partial x_j}$

and c is the concentration of solute $[M/L^3]$;

v_i is the seepage velocity or average pore velocity in the direction of x_i $[L/T]$;

K_{ij} is the hydraulic conductivity tensor $[L/T]$;

h is the hydraulic head $[L]$;

ϕ is the effective porosity of the aquifer [dimensionless];

D_{ij} is the coefficient of hydrodynamic dispersion, a second-order tensor $[L^2T]$;

c' is the concentration of solute in the source or sink fluid $[M/L^3]$;

$W^*=W^*(x_i,t)$ is the volume flux per unit volume (positive sign for outflow and negative for inflow) $[T^{-1}]$;

R_k is the rate of production of the solute in reaction k of s different reactions (positive for addition of solute and negative for removal) $[M/L^3]$;

x_i is the cartesian coordinate system $[L]$;

and t is time $[T]$

The mass-transport equation (10) consists of five terms: the mass accumulation term on the left-hand side of the equation, the dispersion flux term, the convective term, the source/sink term, and the chemical reaction term on the right-hand side of the equation. Because in this study we deal with non-reactive, conservative solutes, the last term on the right-hand side of equation (10) is omitted.

A short description of each of the three selected models for solving equation (10) follow.

Konikow's and Bredehoeft's (1978) method of characteristics (MOC) model: This program uses an iterative alternating direction implicit procedure to solve a finite-difference approximation to the groundwater flow equation in two dimensions, and a method of characteristics to solve the mass-transport equation. The latter consists of a particle-tracking procedure to solve a finite-difference equation that describes the effects of hydrodynamic dispersion, fluid sources and sinks, and divergence of velocity. The dispersion coefficient is treated in its correct tensorial form, but molecular diffusion is neglected. The explicit scheme imposes several stability criteria which are handled automatically by the program. The finite difference grid is rectangular and block-centered. For more details the reader is referred to Konikow and Bredehoeft (1978).

Pinder's and Gray's (Pinder, 1979) finite element model known as ISOQUAD4 (FE): This two-dimensional model is based on Galerkin's approximation in conjunction with mixed (linear to cubic) isoparametric quadrilateral elements. The dispersion coefficient is treated as a full tensor and it includes molecular diffusion. For further details the reader is referred to Pinder (1979).

Grove's (1977) finite difference (FD) model: This program employs the same iterative alternating direction implicit procedure and discretization scheme for solving the groundwater flow equation as the above-mentioned MOC model, but uses an explicit finite difference form when solving for chemical concentrations.

Each of the three models adopted for application were modified to a significant degree in order to make them applicable to the particular requirements of this study. Each model was modified to handle multiple injection and/or pumping periods of different duration; to accommodate multiple sources of different quality waters, such as injection wells or seepage ponds, recharge or seepages of different concentrations; to handle specified boundary conditions in addition to the pre-programmed ones; to handle input-output more easily or efficiently, in addition to a number of other small changes and corrections required during the implementation of these models to the field situation.

BASIC DATA DEFICIENCIES IN MODELING MASS TRANSPORT FOR THE STUDY AREA

As was mentioned previously, 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 poorly 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, 1982, personal communication). This map was verified and supplemented by studying old aerial photos of the area and identifying the disposal ponds. Figure 13 shows the general area of major concentration of disposal ponds, although such ponds also existed to the north of the indicated area. In each section of the indicated area numerous such ponds existed. Such disposal or so-called "evaporation" ponds commonly have an area of 45 to 930 m^2 and a depth of 0.3 to 4.6 m. In most parts of the area where such ponds were used, most of the brine escaped by seepage into the pervious 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 neaby 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

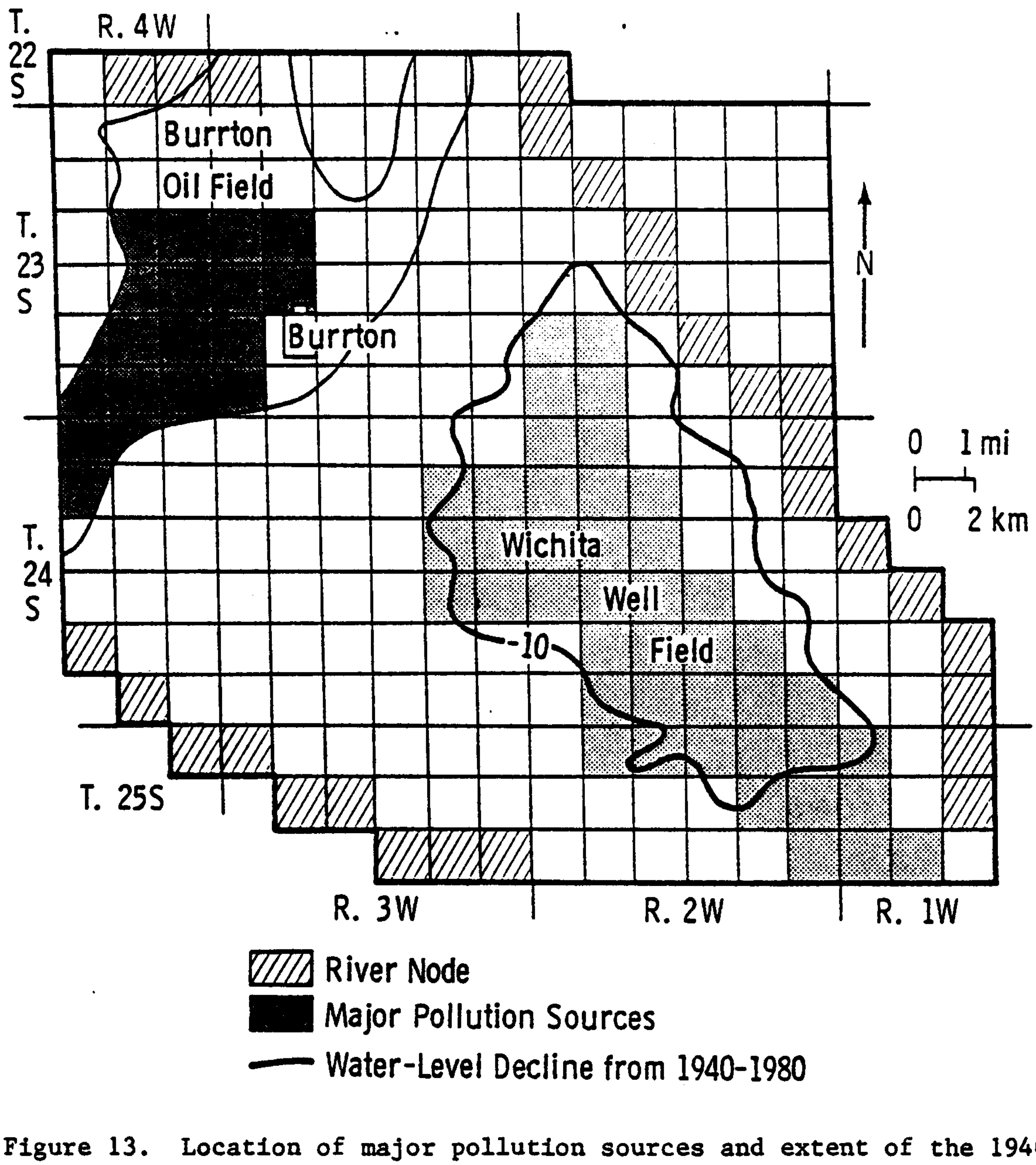

Figure 13. Location of major pollution sources and extent of the 1940-80 three-meter water level areal decline.

state agencies during the 30s and 40s, were completely outlawed by 1957 (Latta, 1963). The life of operation of each of those ponds is practically unknown, although a figure of approximately 10 years seems to be the right order of magnitude (R. O'Connor, 1982, personal communication). 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 100,000 mg/l. 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 fast and was little 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.

COMPARATIVE EVALUATION OF THE CONSIDERED MASS TRANSPORT METHODOLOGIES AND MODELS

Each of the three different methodologies (FD, MOC, and FE) for solving the mass transport equation considered in this study have specific advantages and disadvantages, which will be briefly summarized here. The FD method is mathematically simple, computationally efficient and easy to program. However, it is subject to significant numerical dispersion, especially when the groundwater velocities are large. As with most FD equations, stable solutions occur only with the proper choice of time and space-increment sizes. The choice of a large spatial increment may cause oscillations in the computed concentration matrix (overshoot), especially with small dispersion coefficients. Keller (1967) presented the conditions that are considered sufficient to provide stable nonoscillatory solutions to the finite-difference form of a differential equation describing mass transport. However, depending on the manner of differencing the space and time derivatives, the technique that gives stable solutions may create additional numerical dispersion and overshoot errors. Lantz (1971) calculated the magnitude of the numerical dispersion term for various types of spatial and time increments.

The MOC eliminates numerical dispersion, and is perhaps the best technique for hyperbolic equations. Garder, et al., (1964) attributed the cause of numerical instabilities in solving the mass transport equation by the FD method to the fact that when velocities are large, the mass transport equation behaves like a hyperbolic equation. The MOC is most efficient when the convective term is large relative to the dispersive term. A number of studies have demonstrated the worth of the MOC for modeling two-dimensional mass transport. Konikow and Bredehoeft (1978) present a number of stability criteria for the MOC. The distinctive advantage of this method is the ability to set the dispersion coefficient to zero and to model pure convective flow. Although the MOC gives good results compared to available analytical solutions and is simple in concept, as with any multidimensional model based on the characteristics approach, it is cumbersome to program. Moreover, convergence proofs and error analysis techniques available in other numerical schemes are not generally applicable to the MOC.

The FE method based on a Galerkin approximation has the princpal advantage over the FD and the MOC of being able to represent irregular geometries with a minimum of nodes because it can be used with a mesh composed of subspaces of very general shape, as opposed to rectangles employed in the previous two methods. However, one pays the price of additional complexities in input data preparation. The FE method is conceptually more abstract than the FD method and is more difficult to program, although boundary conditions are often implemented rather easily. Comparisons of FE and FD solutions (Pinder and Gray, 1977) consistently indicate that the FE solutions are more accurate with less apparent numerical dispersion. Moreover, in the FE method one can easily change the order of approximation from one region to another. This approach leads to banded matrices with less regular structure than in the case of FD, with consequent difficulties in employing efficient solution algorithms.

In many instances, FE techniques do not provide a continuous distribution of velocities throughout the discrete model. Although this problem may not be significant when the dispersive term in the mass transport equation predominates, it leads to numerical difficulties, such as negative concentration values, whenever the convective transport term is not negligible.

In summary, there are advantages and disadvantages to each numerical scheme. The scientific literature is replete with comparisons of the numerical performance of the various schemes for solving the mass transport equation and comparing them to available, usually one-dimensional, analytical solutions. Since one of the objectives of this study is also to evaluate several existing numerical schemes for solving the mass transport equation, we decided to do this by comparing the performance of each of the three previously-mentioned numerical methodologies to actual field observations from the Equus Beds aquifer, thus obtaining a more realistic picture of the performance of each scheme.

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. 14), and the locations of surface disposal ponds (Fig. 13) as the sources of contamination, we used all three models with the same regular square grid in our attempts to simulate the water-quality degradation problems of the area and comparatively evaluate the performance of each model. 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 were assigned to the western boundary and along the Arkansas River, while relatively low chloride concentrations (20 mg/l) 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. 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.

Special effort was made to have identical input conditions for all models as far as possible, although such conditions remove some flexibility from the FE model that could approximate any irregular geometry better than the FD or the MOC and could also employ already pre-programmed higher order approximations to the derivatives in the mass transport equation. While in both the FD and the MOC a block-centered discretization scheme is employed, in the FE method a mesh-centered grid is used. For comparison purposes, the four mesh-centered nodes around each block of the FE grid were averaged to get block-centered values. The 1980 predicted chloride concentrations were

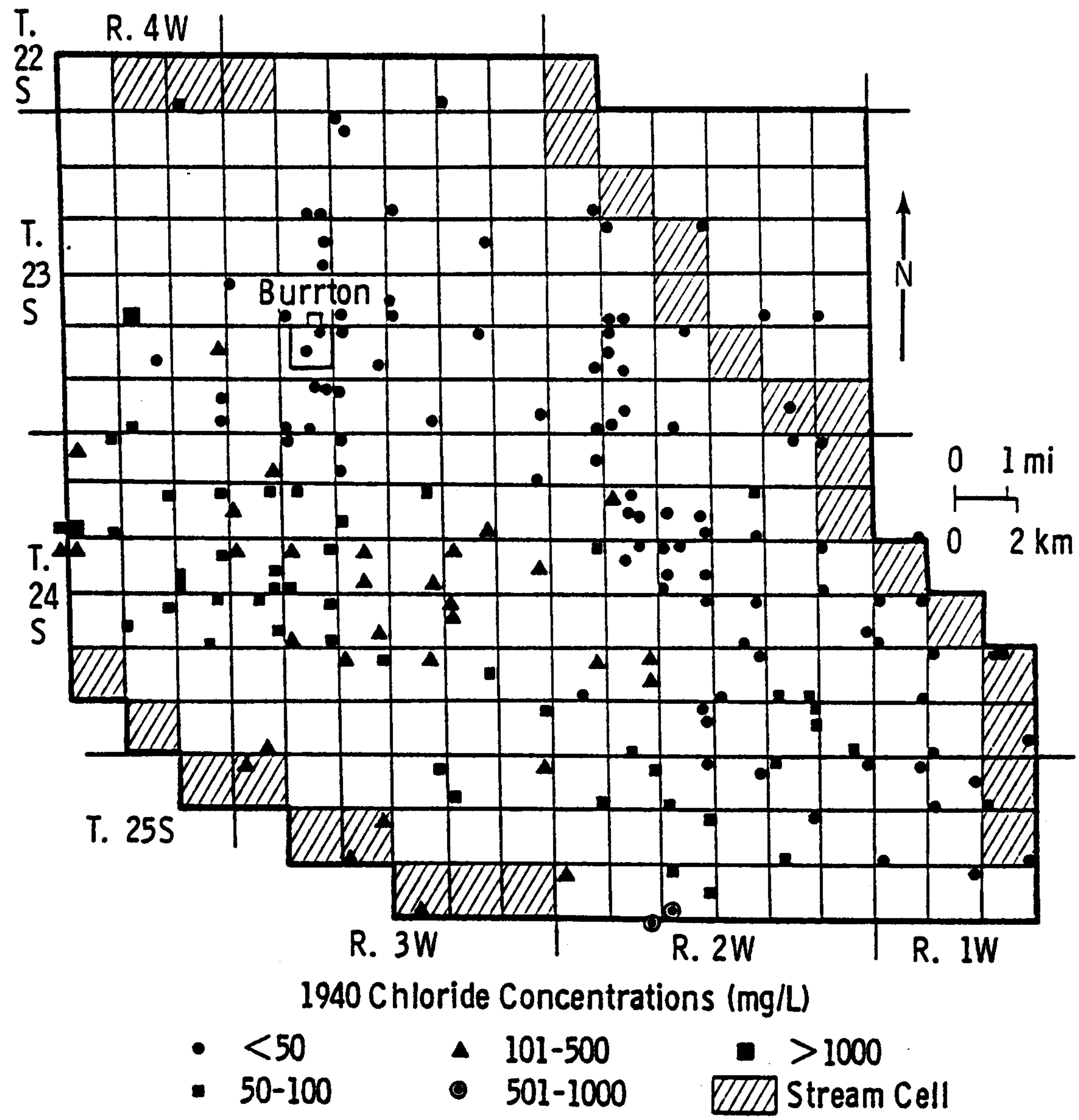

Figure 14. 1940 chloride concentration of groundwater in the study area.

obtained in these models after an initial ten-year continuously active brine-sources period and subsequent 30 years of no-pollution sources simulation were employed. The results of the 1980 chloride concentration simulations are plotted together with the observed 1980 chloride concentrations in Figure 15. The averaging procedure to get block-centered concentration values for the FE program effectively eliminated the few negative values that were simulated in some nodes. The closest approximation to the observed values are marked by an asterisk in the figure. A simultaneous comparison of all three simulated chloride concentrations with the observed values, wherever available, indicates that the MOC most frequently matched the observed data in an overall sense in this particular case study, followed closely by the FE method. If all the closest approximations to the observed chloride values simulated by one or more methods (Fig. 15) are summed up to unity and called successes, then the MOC scored about 44% success, the FE 40%, and the FD 17% in this particular comparison. It should be noted that this comparison is approximate because point values are compared to average block values. These results are not surprising given the predominance of the convective term over the dispersive one in the mass transport equation in this particular case study (refer to the next section for more information related to dispersivity values). Where dispersion predominates over convection, the character of the mass-transport equation is near-parabolic; where convection predominates, its character becomes near-hyperbolic, as is the case here. In such cases, as stated previously, a method of characteristics-type approach will probably perform better than the FD or FE approach. The execution time for these simulations were 0.01 hours for the MOC, 0.04 hours for the FD and 0.13 hours for the FE method using the Honeywell 66/60 computer system of The University of Kansas. From a practical point of view, the input to both FD and MOC models is much easier to handle and the output much easier to interpret than are the input and output of the FE model dealt with here. As a result of this preliminary comparison, the MOC approach is adopted for subsequent analysis.

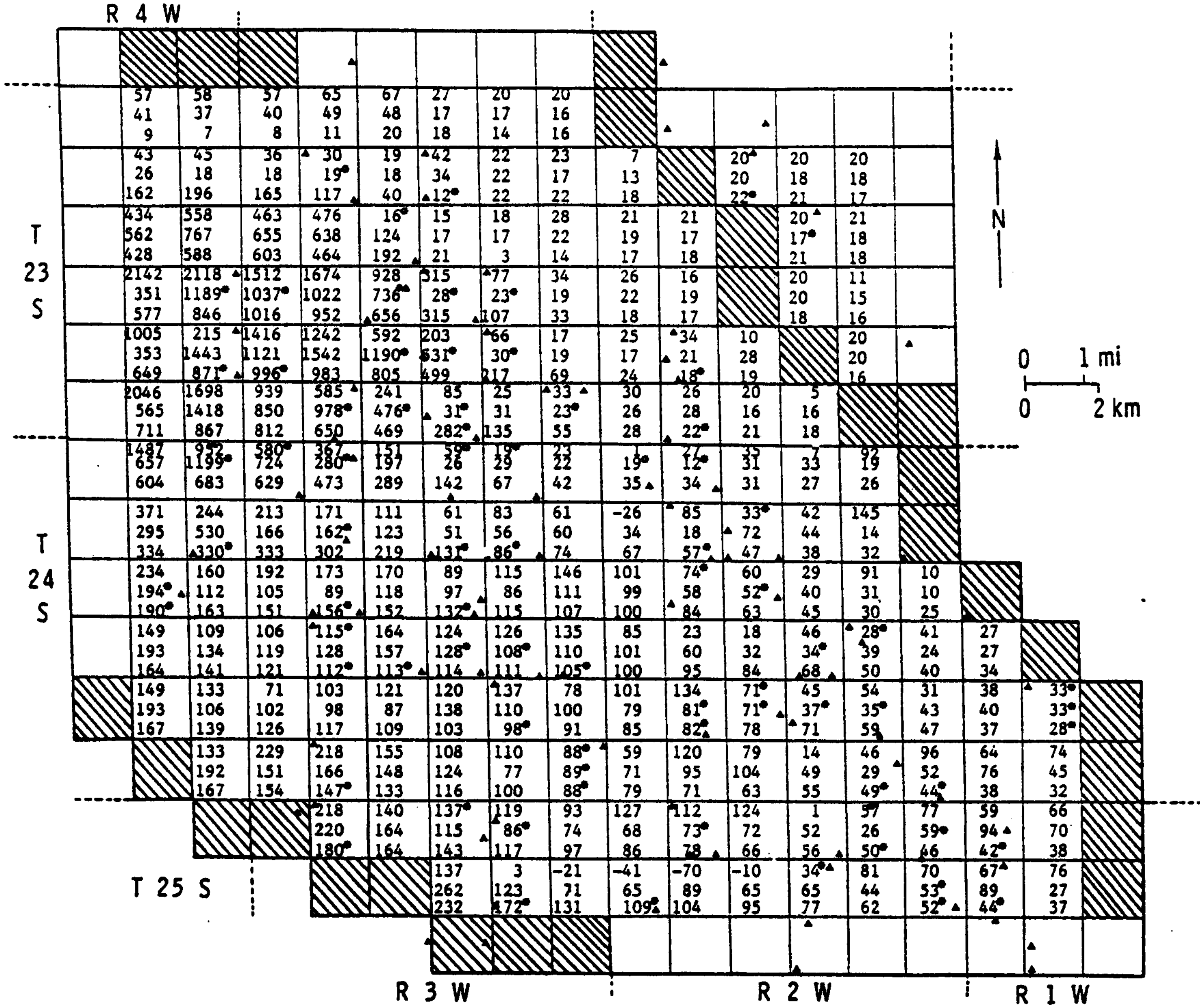

Figure 15. Simultaneous comparison of the 1980 chloride distribution (mg/l) simulated by a finite difference model (top number), a method of characteristics model (middle number), and a finite element model (bottom number). Solid triangles indicate actually measured chloride concentrations during 1980, which are shown in Figure 18. See text for further explanation.

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. 16) 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 years of simulation. Some of the results are shown in Figure 16 for the greater-than-1000 mg/l chloride concentration. The complete simulation results are shown in Appendix A. 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 40s, 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. Figure 17 shows the results of

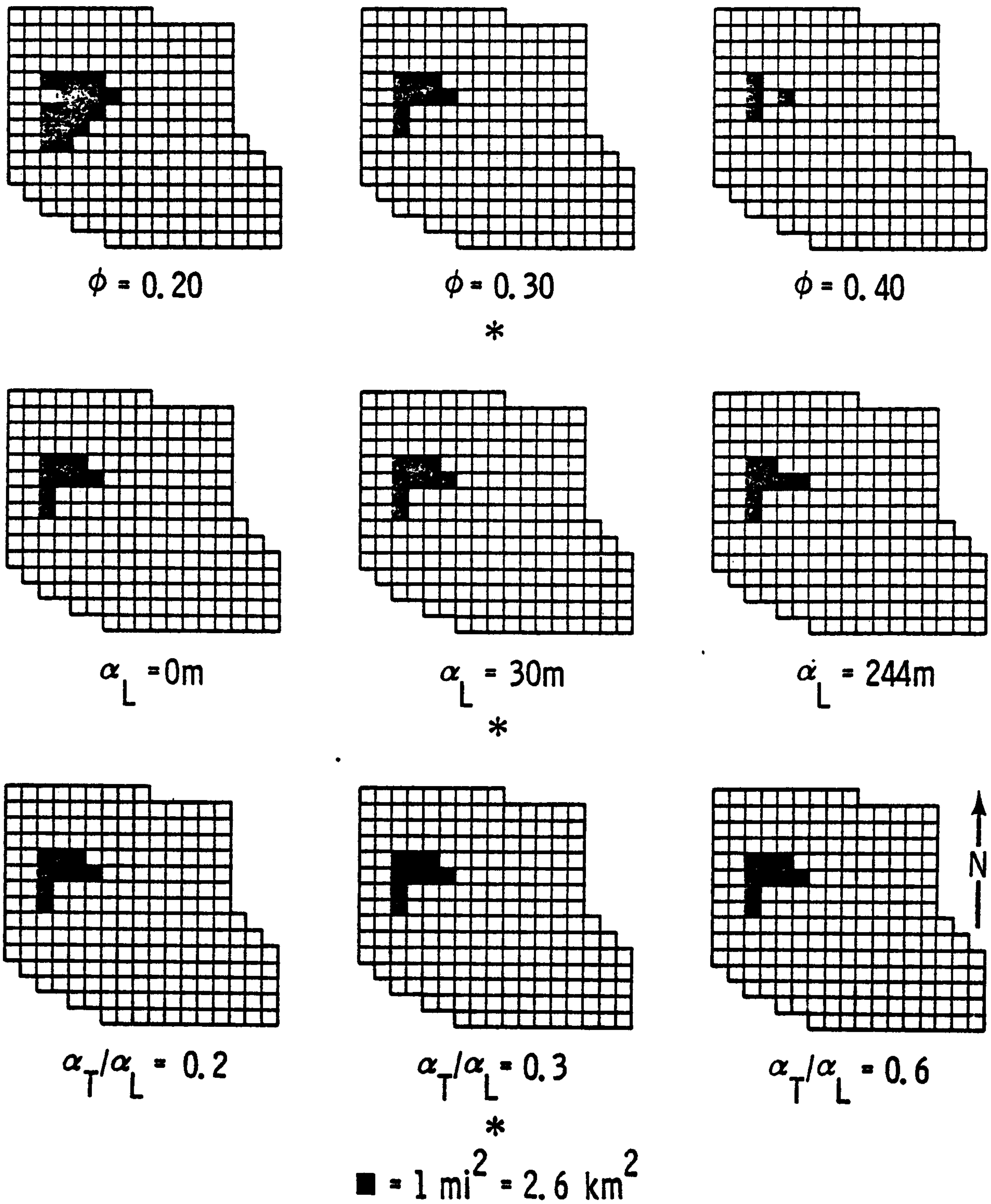

Figure 16. Model sensitivity to various parameters as indicated by the greater than 1000 mg/l chloride distribution after 40 years of simulation. An asterisk indicates the adopted parameter value.

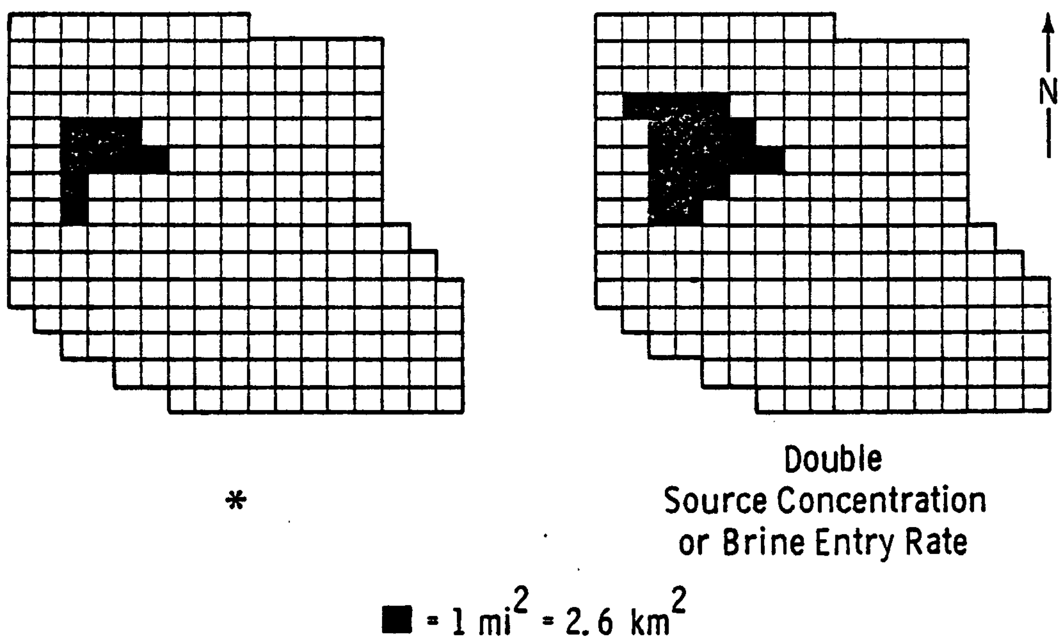

Figure 17. Effects of doubling the rate of seepage or the concentration of the percolating oil-field brine on the greater than 1000 mg/l chloride distribution after 40 years of simulation.

doubling the rate of seepage or the concentration in the percolating water. Of course 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 Figure 18. The match between observed and calculated results seems to be satisfactory, given that the model predicts average concentrations over a square-mile area. Once a match to the historical data was obtained, chloride concentration projections for the year 2000, as indicated by the greater-than-1000 mg/l chloride distribution, were made (Fig. 19). A detailed prediction of the chloride concentration distribution for the year 2000, together with the initial and present chloride distributions, are shown in Appendix B. This projection shows that the brine plume, in a relatively diluted form, would barely reach to within a mile of the westernmost edge of the Wichita well field by the year 2000. Because the cone of depression caused by the Wichita well field pumpage, as indicated by the three-meter 1940-1980 water-level decline contour (Fig. 13), has not yet been extended significantly beyond the boundaries of the well field, we believe that the results of the present simulation are valid.

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.

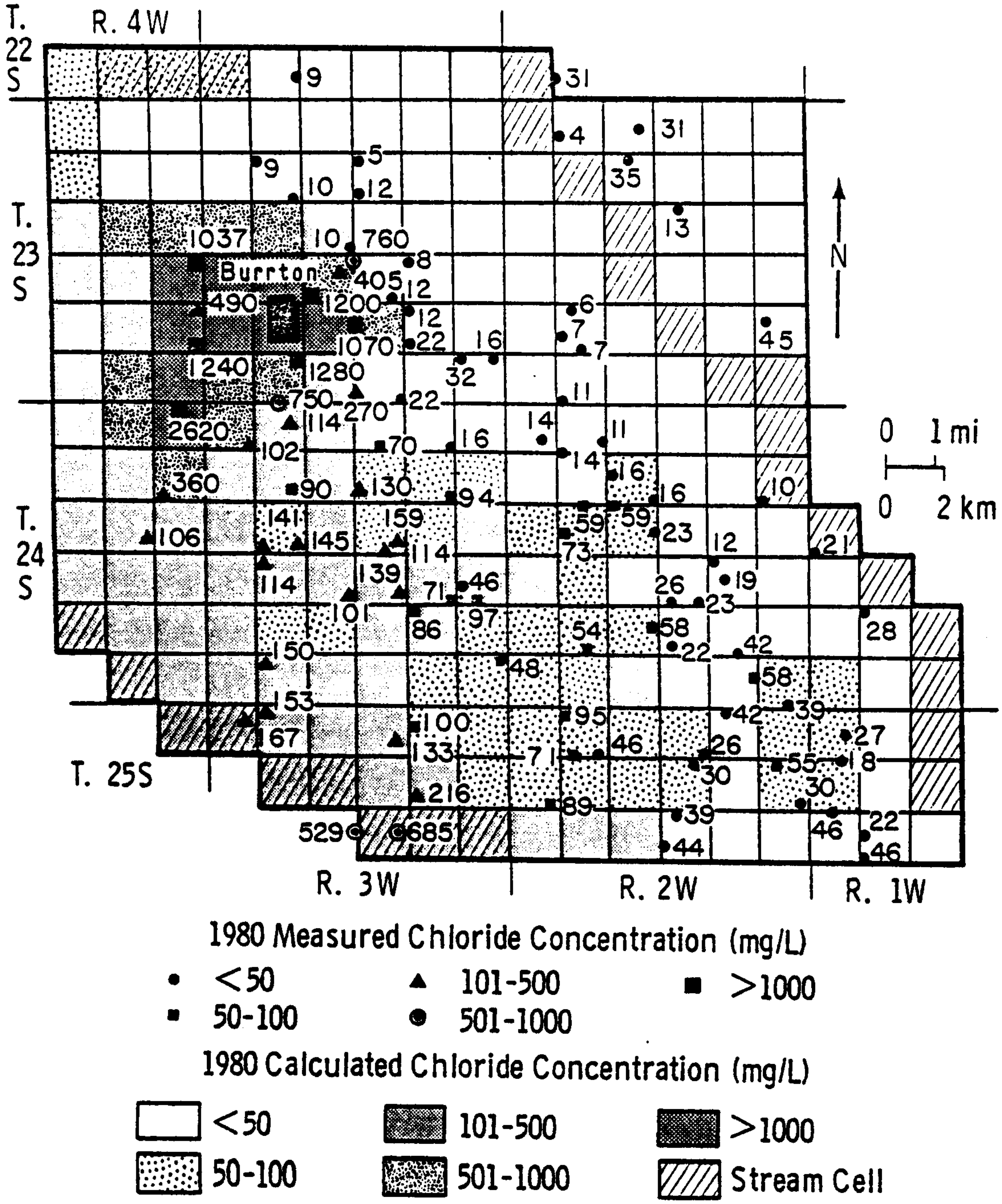

Figure 18. Comparison of measured and simulated chloride concentrations.

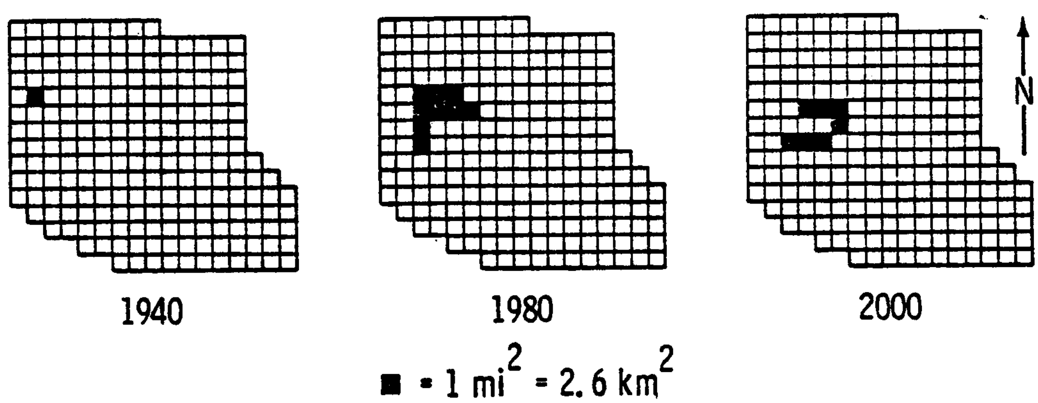

Figure 19. Historic evolution and future projection of the greater than 1000 mg/l chloride concentration.

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) A simultaneous comparison of three different methodologies for modeling groundwater quality problems as applied to the study area indicated 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 is a better approach to follow as compared to the finite difference and finite element approaches considered in this study.

4) 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.

5) 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. However, the brine plume is shown to be moving southeastwards in a relatively diluted form (Fig. 18), but still rendering the chloride concentration of groundwaters in that general direction above the recommended drinking limits. Therefore, it would be prudent to continue salt-water monitoring efforts.

6) The predictive capability of the model can be helpful in expanding the present salt-water 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.

APPENDIX A

APPENDIX A: CHLORIDE CONCENTRATION OUTPUTS FOR VARIOUS MASS-TRANSPORT PARAMETERS AFTER 40 YEARS OF SIMULATION

Note: In all chloride concentration outputs that follow, the value characterizing the section where the town of Burrton is located is outlined by a rectangle. Each indicated value represents the chloride concentration at the center of a 2.6 km^2 (1 mi^2 or section) square block. Some common execution parameters used to produce the outputs presented in this appendix are:

NPTPND (initial number of particles per node) = 9
CELDIS (maximum cell distance per move of particles in one step as a fraction of grid dimensions) = 0.5

65	65	65	65	20	20	20	20	20	20	0	0	0	0	0	0	0	0
65	42	29	31	30	29	23	19	15	20	20	20	20	20	20	0	0	0
65	30	18	18	19	17	27	21	16	14	20	20	18	18	20	0	0	0
365	463	939	876	825	345	16	16	19	18	15	11	16	17	20	0	0	0
365	443	1186	1421	1047	1029	996	40	20	20	20	20	20	14	13	0	0	0
365	359	980	1539	$\boxed{1805}$	1910	1312	145	25	17	17	18	20	20	20	0	0	0
478	461	1288	1431	1380	1426	244	43	34	21	27	24	24	20	20	0	0	0
478	470	1600	1692	1336	758	240	31	27	19	20	11	37	30	11	0	0	0
200	239	1028	1208	195	184	126	28	43	51	19	17	94	15	20	0	0	0
200	191	137	87	91	116	114	83	73	103	66	37	64	46	10	20	0	0
200	191	175	161	109	101	126	109	98	123	87	51	30	36	38	27	20	0
200	191	123	66	90	89	129	124	102	97	70	73	41	32	35	38	33	20
0	200	192	163	120	115	98	125	90	81	68	126	104	20	35	44	57	20
0	0	200	200	205	220	127	114	73	84	68	69	82	27	21	59	98	20
0	0	0	0	365	365	298	166	102	69	66	79	52	65	12	50	90	20
0	0	0	0	0	0	500	365	365	365	365	240	40	40	40	20	30	20

Parameters: $\phi = 0.2$ $\alpha_L = 30$ m (100 ft) $\alpha_T/\alpha_L = 0.3$

65	65	65	65	20	20	20	20	20	20	0	0	0	0	0	0	0	0
65	41	37	40	49	48	17	17	16	20	20	20	20	20	20	0	0	0
65	26	18	18	19	18	34	22	17	13	20	20	18	18	20	0	0	0
365	562	767	655	638	124	17	17	22	19	17	11	17	18	20	0	0	0
365	351	1189	1037	1022	736	28	23	19	22	19	20	20	15	13	0	0	0
365	353	1443	1121	$\boxed{1542}$	1190	531	30	19	17	21	28	20	20	20	0	0	0
478	565	1418	850	978	476	31	31	23	26	28	16	16	20	20	0	0	0
478	657	1199	724	280	197	26	29	22	19	12	31	33	19	11	0	0	0
200	295	530	166	162	123	51	56	60	34	18	72	44	14	20	0	0	0
200	194	112	105	89	118	97	86	111	99	58	52	40	31	10	20	0	0
200	193	134	119	128	157	128	108	110	101	60	32	34	39	24	27	20	0
200	193	106	102	98	87	138	110	100	79	81	71	37	35	43	40	33	20
0	200	192	151	166	148	124	77	89	71	95	104	49	29	52	76	45	20
0	0	200	200	220	164	115	86	74	68	73	72	52	26	59	94	70	20
0	0	0	0	365	365	262	123	71	65	89	65	65	44	53	89	27	20
0	0	0	0	0	0	500	365	365	365	365	240	40	40	40	20	30	20

Parameters: $\phi = 0.3$ $\alpha_L = 30$ m (100 ft) $\alpha_T/\alpha_L = 0.3$

65	65	65	65	20	20	20	20	20	20	0	0	0	0	0	0	0	0
65	44	53	54	52	52	18	17	17	20	20	20	20	20	20	0	0	0
65	18	19	19	19	18	36	18	18	11	20	20	18	19	20	0	0	0
365	652	622	515	520	19	18	18	24	20	17	11	18	19	20	0	0	0
365	581	1185	940	910	656	24	14	20	20	19	20	20	14	13	0	0	0
365	552	1076	913	$\boxed{1056}$	608	96	29	13	19	26	20	20	20	20	0	0	0
478	680	1124	668	542	46	30	31	17	38	19	15	11	20	20	0	0	0
478	801	931	410	211	59	31	29	20	17	10	45	19	20	11	0	0	0
200	299	356	131	130	98	52	59	66	18	20	102	15	91	20	0	0	0
200	179	142	103	116	124	99	88	131	87	45	58	31	42	10	20	0	0
200	166	101	111	132	139	125	105	119	90	46	25	38	33	27	27	20	0
200	179	140	104	105	124	131	105	94	72	104	81	25	41	45	42	33	20
0	200	190	154	183	133	101	84	85	73	99	96	25	28	73	67	33	20
0	0	200	200	231	140	120	95	69	72	72	71	48	16	104	73	55	20
0	0	0	0	365	365	300	90	68	78	97	62	72	30	79	52	32	20
0	0	0	0	0	0	500	365	365	365	365	240	40	40	40	20	30	20

Parameters: $\phi = 0.4$ $\alpha_L = 30$ m (100 ft) $\alpha_T/\alpha_L = 0.3$

65	65	65	65	20	20	20	20	20	20	0	0	0	0	0	0	0	0
65	41	37	40	49	49	17	17	16	20	20	20	20	20	20	0	0	0
65	24	17	17	17	17	34	22	17	12	20	20	18	18	20	0	0	0
365	561	764	653	638	122	17	17	22	19	17	11	17	18	20	0	0	0
365	347	1202	1041	1029	745	20	19	19	22	19	20	20	15	13	0	0	0
365	349	1460	1119	$\boxed{1561}$	1207	526	23	19	16	21	28	20	20	20	0	0	0
478	565	1439	848	989	469	22	31	22	26	28	15	16	20	20	0	0	0
478	663	1215	717	270	190	21	29	21	19	11	32	34	19	11	0	0	0
200	295	527	158	154	121	48	56	61	33	16	75	43	13	20	0	0	0
200	194	110	102	86	118	96	86	112	101	58	53	40	31	10	20	0	0
200	193	133	117	128	160	128	108	111	101	59	31	34	39	24	27	20	0
200	193	104	101	97	86	140	110	100	78	81	72	37	35	43	40	33	20
0	200	192	151	167	149	125	76	90	70	96	106	49	27	53	77	45	20
0	0	200	200	220	162	113	85	74	67	74	72	51	24	60	97	71	20
0	0	0	0	365	365	261	120	67	61	87	63	66	44	54	92	26	20
0	0	0	0	0	0	500	365	365	365	365	240	40	40	40	20	30	20

Parameters: $\phi = 0.3$ $\alpha_L = 0$ m $\alpha_T/\alpha_L = 0$

65	65	65	65	20	20	20	20	20	20	0	0	0	0	0	0	0	0
65	43	38	41	48	47	17	17	16	20	20	20	20	20	20	0	0	0
65	31	22	21	22	18	34	22	17	13	20	20	18	18	20	0	0	0
365	565	774	663	637	130	16	17	21	19	17	11	17	18	20	0	0	0
365	362	1153	1024	1000	713	50	35	19	21	19	20	20	15	13	0	0	0
365	366	1391	1123	$\boxed{1487}$	1142	540	51	21	18	20	26	20	20	20	0	0	0
478	562	1358	856	947	494	61	34	24	25	27	17	17	20	20	0	0	0
478	641	1151	739	308	216	42	30	23	19	14	30	32	21	11	0	0	0
200	295	534	190	185	130	57	57	59	36	22	65	47	17	20	0	0	0
200	195	119	114	99	118	99	87	107	96	59	51	41	32	10	20	0	0
200	193	137	122	129	151	127	108	109	99	62	36	35	38	24	27	20	0
200	193	110	105	102	90	133	110	99	81	80	68	39	35	43	39	33	20
0	200	191	153	164	145	123	80	88	74	94	99	51	32	51	71	44	20
0	0	200	200	220	168	121	89	76	70	74	72	52	31	56	87	68	20
0	0	0	0	365	365	264	133	84	77	93	70	64	45	51	83	31	20
0	0	0	0	0	0	500	365	365	365	365	240	40	40	40	20	30	20

Parameters: $\phi = 0.3$ $\alpha_L = 122$ m (400 ft) $\alpha_T/\alpha_L = 0.3$

65	65	65	65	20	20	20	20	20	20	0	0	0	0	0	0	0	0
65	45	39	41	46	45	18	17	16	20	20	20	20	20	20	0	0	0
65	38	27	25	26	18	33	21	17	14	20	20	18	18	20	0	0	0
365	568	783	673	636	137	16	17	21	19	16	11	17	18	20	0	0	0
365	378	1110	1005	972	686	74	50	21	21	19	20	20	15	13	0	0	0
365	383	1326	1120	$\boxed{1421}$	1084	548	78	25	19	20	24	20	20	20	0	0	0
478	560	1283	861	910	513	98	39	25	24	26	18	17	20	20	0	0	0
478	622	1091	750	341	239	63	32	24	20	17	29	31	22	11	0	0	0
200	295	534	220	213	141	66	58	57	38	26	57	48	20	20	0	0	0
200	195	128	126	112	120	101	88	102	91	59	50	42	32	10	20	0	0
200	192	140	126	130	144	126	109	107	97	64	40	36	38	25	27	20	0
200	193	116	108	106	94	128	109	99	83	79	65	40	36	42	37	33	20
0	200	191	155	161	143	122	84	88	77	91	94	53	36	49	65	44	20
0	0	200	200	220	173	128	93	78	72	74	72	53	36	54	79	64	20
0	0	0	0	365	365	268	146	100	92	99	76	63	46	49	75	34	20
0	0	0	0	0	0	500	365	365	365	365	240	40	40	40	20	30	20

Parameters: $\phi = 0.3$ $\alpha_L = 244$ m (800 ft) $\alpha_T/\alpha_L = 0.3$

65	65	65	65	20	20	20	20	20	20	0	0	0	0	0	0	0	0
65	41	37	40	49	48	17	17	16	20	20	20	20	20	20	0	0	0
65	26	18	18	18	18	34	22	17	13	20	20	18	18	20	0	0	0
365	563	766	655	637	123	17	17	22	19	17	11	17	18	20	0	0	0
365	351	1190	1038	1023	736	28	23	19	22	19	20	20	15	13	0	0	0
365	353	1443	1121	$\boxed{1543}$	1192	532	30	19	17	21	28	20	20	20	0	0	0
478	565	1419	850	978	476	31	31	23	26	28	16	16	20	20	0	0	0
478	658	1200	724	279	197	26	29	21	19	12	31	33	19	11	0	0	0
200	295	529	166	162	123	50	56	60	34	18	72	44	14	20	0	0	0
200	194	111	105	89	118	97	86	111	100	59	52	40	31	10	20	0	0
200	193	134	118	128	158	128	108	110	101	60	32	34	39	24	27	20	0
200	193	106	102	98	87	138	110	100	79	81	71	37	35	43	40	33	20
0	200	192	151	166	148	124	77	89	71	95	104	49	29	52	76	45	20
0	0	200	200	220	164	115	86	74	68	73	72	52	26	59	95	70	20
0	0	0	0	365	365	262	123	70	65	88	64	65	44	53	90	27	20
0	0	0	0	0	0	500	365	365	365	365	240	40	40	40	20	30	20

Parameters: $\phi = 0.3$ $\alpha_L = 30$ m (100 ft) $\alpha_T/\alpha_L = 0.2$

65	65	65	65	20	20	20	20	20	20	0	0	0	0	0	0	0	0
65	41	37	40	49	48	17	17	16	20	20	20	20	20	20	0	0	0
65	26	19	19	19	18	34	22	17	13	20	20	18	18	20	0	0	0
365	561	767	657	639	127	18	17	22	19	17	11	17	18	20	0	0	0
365	351	1186	1035	1021	736	29	23	19	22	19	20	20	15	13	0	0	0
365	354	1443	1120	$\boxed{1538}$	1185	528	29	19	17	21	28	20	20	20	0	0	0
478	564	1416	851	978	479	32	31	23	26	28	16	16	20	20	0	0	0
478	656	1196	723	282	198	26	29	22	19	12	31	33	20	11	0	0	0
200	297	533	167	163	123	51	56	61	34	18	71	44	14	20	0	0	0
200	195	113	105	89	118	97	86	110	99	58	52	40	31	10	20	0	0
200	193	134	119	128	157	128	108	110	101	60	33	34	39	24	27	20	0
200	193	106	103	99	88	138	110	100	79	81	71	37	35	43	40	33	20
0	200	192	151	166	148	125	77	89	71	95	103	49	29	52	75	45	20
0	0	200	200	220	164	116	87	75	68	74	72	52	26	59	94	70	20
0	0	0	0	365	365	262	124	73	66	90	66	66	44	53	89	27	20
0	0	0	0	0	0	500	365	365	365	365	240	40	40	40	20	30	20

Parameters: $\phi = 0.3$ $\alpha_L = 30$ m (100 ft) $\alpha_T/\alpha_L = 0.6$

APPENDIX B

APPENDIX B: MODEL OUTPUTS FOR INITIAL (1940), PRESENT (1980), AND FUTURE (YEAR 2000) CHLORIDE CONCENTRATIONS

<u>Note</u>: In all chloride concentration outputs that follow, the value characterizing the section where the town of Burrton is located is outlined by a rectangle. Each indicated value represents the chloride concentration at the center of a 2.6 km^2 (1 mi^2 or section) square block. Some common execution parameters used to produce the outputs presented in this appendix are:

NPTPND (initial number of particles per node) = 9
CELDIS (maximum cell distance per move of particles in one step as a fraction of grid dimensions) = 0.5

65	65	65	65	20	20	20	20	20	20	0	0	0	0	0	0	0	0
65	65	65	65	65	66	20	20	20	20	20	20	20	20	20	0	0	0
65	20	20	20	20	20	43	20	20	6	20	20	20	20	20	0	0	0
365	75	70	20	20	22	20	20	29	20	20	11	20	20	20	0	0	0
365	1825	20	7	20	13	6	20	20	20	13	20	20	11	13	0	0	0
365	18	218	20	20	44	44	11	20	33	8	9	20	20	20	0	0	0
478	58	26	20	19	27	26	20	40	16	15	7	20	20	20	0	0	0
478	140	200	138	19	49	26	20	14	10	48	20	20	20	11	0	0	0
200	87	90	136	100	92	73	94	20	20	111	14	99	20	20	0	0	0
200	180	135	183	139	128	100	163	128	61	37	44	20	20	10	20	0	0
200	68	95	97	160	124	110	110	77	41	20	38	44	20	39	27	20	0
200	200	140	140	140	86	107	79	75	145	118	20	42	69	20	32	33	20
0	200	200	308	150	100	75	75	85	75	92	28	20	121	78	20	34	20
0	0	200	200	140	200	76	66	123	78	52	73	10	100	28	41	5	20
0	0	0	0	365	365	200	140	140	75	75	84	75	58	40	33	20	20
0	0	0	0	0	0	500	365	365	365	365	240	40	40	40	20	30	20

Initial (1940) chloride concentrations (mg/l)

65	65	65	65	20	20	20	20	20	20	0	0	0	0	0	0	0	0
65	41	37	40	49	48	17	17	16	20	20	20	20	20	20	0	0	0
65	26	18	18	19	18	34	22	17	13	20	20	18	18	20	0	0	0
365	562	767	655	638	124	17	17	22	19	17	11	17	18	20	0	0	0
365	351	1189	1037	1022	736	28	23	19	22	19	20	20	15	13	0	0	0
365	353	1443	1121	$\boxed{1542}$	1190	531	30	19	17	21	28	20	20	20	0	0	0
478	565	1418	850	978	476	31	31	23	26	28	16	16	20	20	0	0	0
478	657	1199	724	280	197	26	29	22	19	12	31	33	19	11	0	0	0
200	295	530	166	162	123	51	56	60	34	18	72	44	14	20	0	0	0
200	194	112	105	89	118	97	86	111	99	58	52	40	31	10	20	0	0
200	193	134	119	128	157	128	108	110	101	60	32	34	39	24	27	20	0
200	193	106	102	98	87	138	110	100	79	81	71	37	35	43	40	33	20
0	200	192	151	166	148	124	77	89	71	95	104	49	29	52	76	45	20
0	0	200	200	220	164	115	86	74	68	73	72	52	26	59	94	70	20
0	0	0	0	365	365	262	123	71	65	89	65	65	44	53	89	27	20
0	0	0	0	0	0	500	365	365	365	365	240	40	40	40	20	30	20

Present (1980) chloride concentrations (mg/l)

65	65	65	65	20	20	20	20	20	20	0	0	0	0	0	0	0	0
65	42	29	31	30	31	16	19	15	20	20	20	20	20	20	0	0	0
65	30	17	18	18	17	27	21	16	14	20	20	18	17	20	0	0	0
365	355	629	560	542	234	16	16	19	18	15	11	16	17	20	0	0	0
365	395	739	845	779	693	369	34	20	20	21	20	20	14	13	0	0	0
365	358	648	1383	$\boxed{1297}$	1348	897	132	24	17	17	18	20	20	20	0	0	0
478	457	756	856	813	1164	358	41	34	21	27	24	24	20	20	0	0	0
478	467	1179	1384	1008	409	166	30	27	19	20	11	37	30	11	0	0	0
200	216	540	772	167	178	123	27	43	51	18	17	94	15	20	0	0	0
200	191	134	83	86	113	114	88	73	103	66	37	64	46	10	20	0	0
200	191	174	160	109	101	127	109	98	123	87	51	30	36	38	27	20	0
200	191	124	66	90	89	129	124	102	97	70	73	41	32	35	38	33	20
0	200	192	163	120	115	98	125	91	81	68	126	105	20	35	44	58	20
0	0	200	200	210	220	127	113	73	84	68	69	82	27	21	59	98	20
0	0	0	0	365	365	272	132	101	69	66	79	52	65	12	51	90	20
0	0	0	0	0	0	500	365	365	365	365	240	40	40	40	20	30	20

Predicted (year 2000) chloride concentrations (mg/l)

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