HYDROGEOCHEMICAL INTERPRETATION AND COMPUTER SIMULATION OF THE SUNDRE AQUIFER, MINOT, NORTH DAKOTA

By

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PREFACE

The Sundre aquifer was studied in order to determine the source of the sulfate, which occurs in concentrations over 1,000 mg/l. An analytical version of the solute-transport model "Random-Walk" was used to simulate the movement of sulfate in the Sundre aquifer. The sulfate was determined to be the result of the oxidation of organic sulfides, present in the till which mantles the bedrock. The analytical version of the solute-transport model was not capable of predicting sulfate levels in the Sundre well field.

I would like to thank my adviser, Dr. Arthur Hounslow, for his support and guidance during this research project. Committee members Dr. Wayne Pettyjohn and Dr. Gary Stewart also provided guidance, for which I am very grateful. Assistance on the computer model was provided by Mr. Kelly Goff.

For their support and encouragement, I would like to thank my friends and family.

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CHAPTER I

INTRODUCTION

Purpose

The purpose of the research described here was to study the hydrogeochemistry of the Sundre aquifer and to evaluate the operation of the solute-transport model "Random-Walk" with respect to the Sundre aquifer.

The city of Minot, North Dakota completed five large-capacity production wells in the Sundre aquifer in 1974 and 1975. Chemical analyses of water from each well at the time of completion revealed sulfate levels of 250 mg/l or less. The next analyses available to me, taken in 1978, indicated the sulfate level had increased to 670 mg/l in the E well. It is the specific purpose of this report to characterize the source of the sulfate ions and evaluate the potential for mixing of waters within the aquifer. The conceptual model produced through this investigation forms the foundation for the computer simulation. The solute-transport model was evaluated as to its ability to simulate movement of sulfate within the Sundre aquifer.

Location

The area of investigation is located in the northwestern part of the Drift Prairie District of the Central Lowlands physiographic province of North Dakota, (figure 1). The city of Minot, North Dakota lies approximately six miles to the northwest of the study area. The Souris River flows through the study area to the southeast. The legal description for the study area is sections 1-12, Township 154 north, Range 82 west.

Location Numbering System

The public land grid system of the United States Bureau of Land Management is used to locate wells and test holes. The first numeral indicates the township, north of a base line in Arkansas. The second numeral denotes the range west of the fifth principal meridian. The section in which the well is located is indicated by the third numeral. Letters are used to indicate the location within the section. Letters a, b, c, and d represent, respectively, the northeast, northwest, southwest, and southeast quarter section. Multiple letters are used to indicate quarter-quarter section and quarter-quarter-quarter section (10 acre tract). A diagrammatic explanation is presented in figure 2.

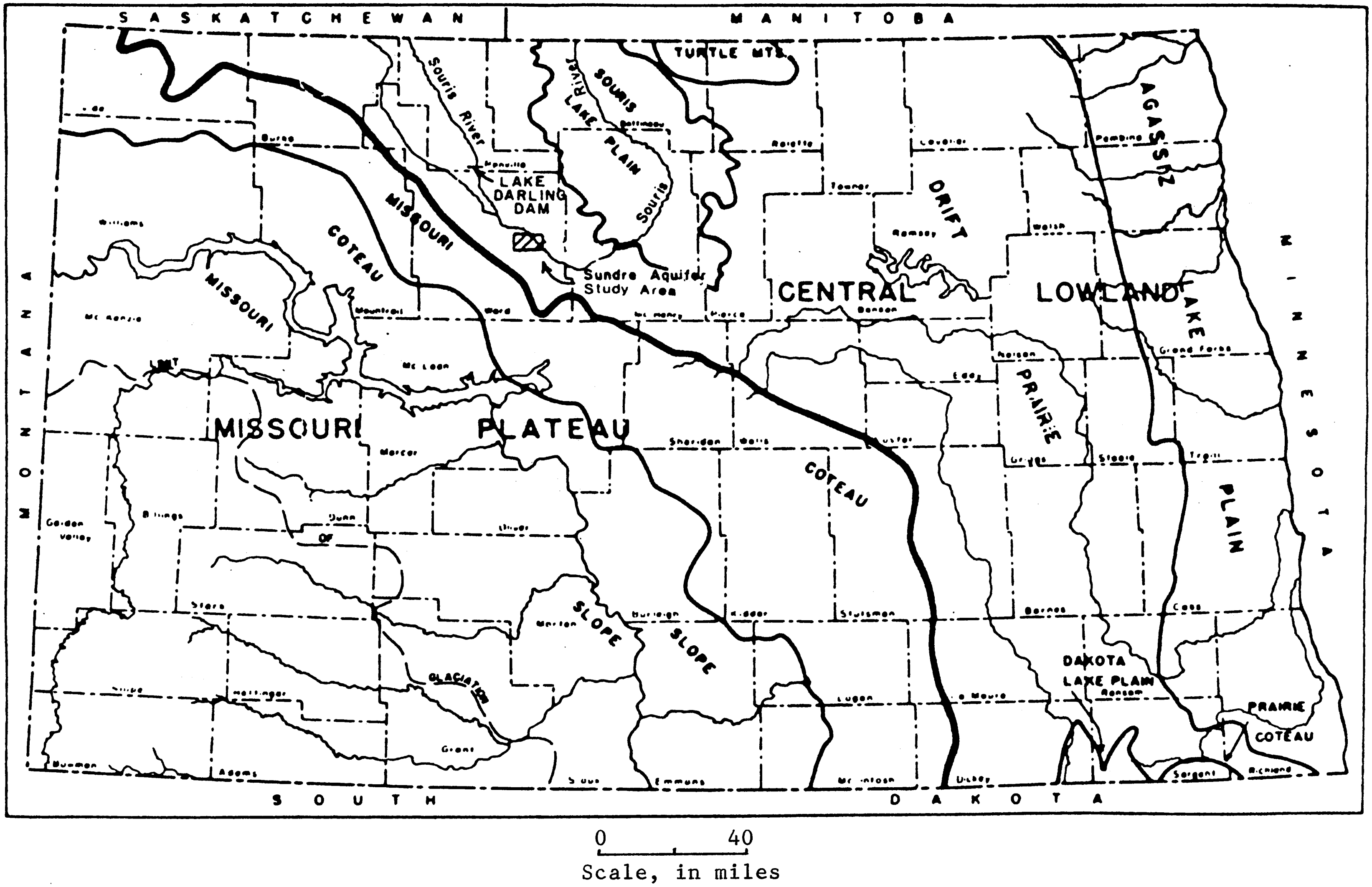


Figure 1. Map Showing Physiographic Provinces of North Dakota and Location of Study Area (modified from Clayton, 1962)

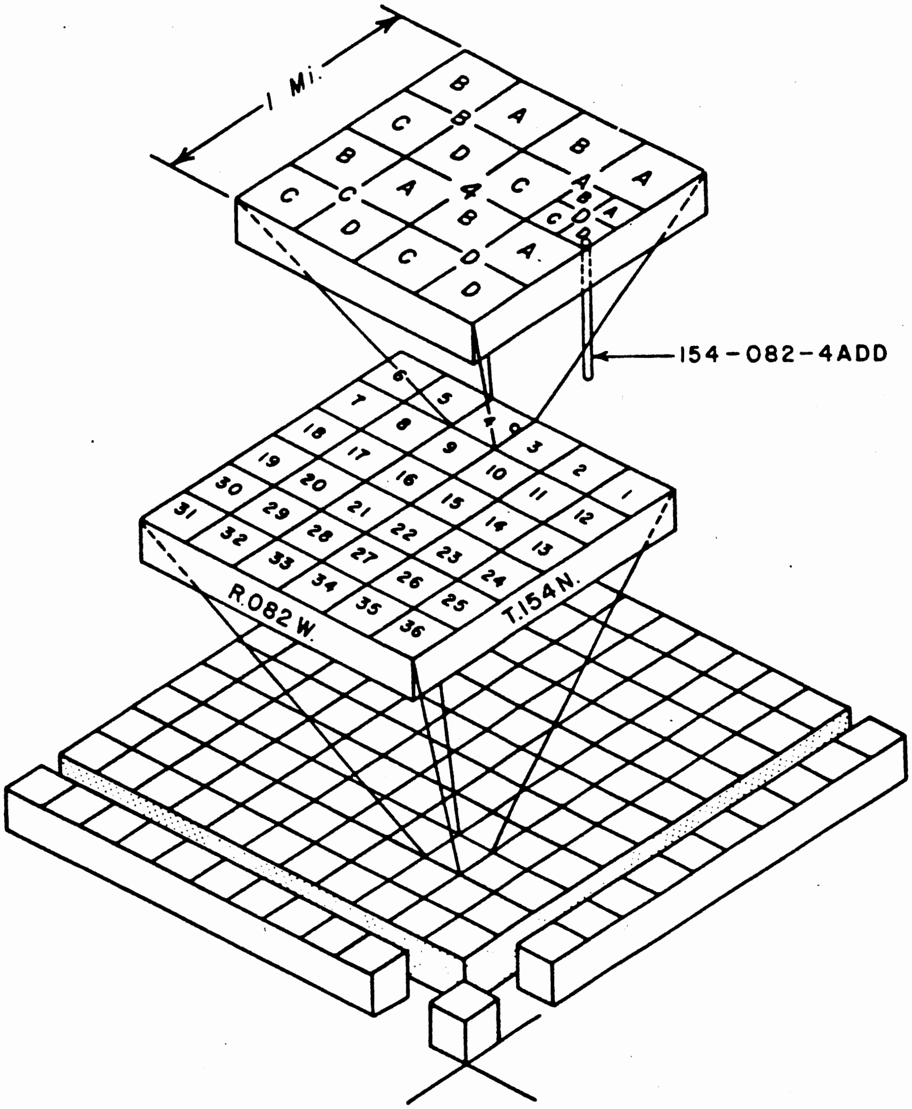


Figure 2. Well-Location Numbering System

CHAPTER II

PREVIOUS INVESTIGATIONS

The earliest geological investigation in the area was conducted by Simpson in 1929. He described the general geology and ground water occurrences in North Dakota. Included in Simpson's report were geologic logs and chemical analyses of water samples taken from wells producing from bedrock and glacial deposits. Akin (1947) prepared a report on the geology and ground-water condictions specifically for the Minot area, included were detailed records of Minot's surface-water and ground-water supplies from 1900 to 1947. Bradley (1963) detailed the interactions between surface water and ground water in the Souris River valley near Minot.

A two part report by Pettyjohn and Hills (1965) and Pettyjohn (1967) discussed the geohydrology of the Souris River valley near Minot. The first part contained data collected in 1963 and 1964, which included sample log descriptions, ground-water quality data and locations for all water wells and test holes in the area of investigation. Pettyjohn (1967), in the second part, reported on the hydrology and chemical quality of the Minot aquifer.

The Sundre buried channel was discovered during this investigation. Pettyjohn suggested further drilling to define the limits of the Sundre aquifer and an aquifer test to evaluate future development potential.

The geology and ground-water resources of Renville and Ward counties were described by Pettyjohn (1968), and Pettyjohn and Hutchinson (1971). The first report contained basic data used in the study, with the second report detailing the regional hydrogeology of the two county area.

Pettyjohn (1970) conducted a detailed aquifer test for the Sundre aquifer. An ongoing evaluation of water level trends during the development of the Sundre aquifer was recommended.

The geologic and hydrogeologic conditions affecting construction and waste disposal in the Minot area were discussed by Kehew (1983). Depositional environments of buried-valley aquifers in North Dakota were investigated by Kehew and Boettger (1986), and Kehew and Lord (1986).

The hydrogeochemistry and rock-water interactions were reported on by Wheatcraft (1987). Isolated gypsum deposits were suggested as the source for high sulfate levels, with the gypsum acting as a catalyst species in dedolomitization reactions.

Poore (1987) reported on the hydrogeology of the Sundre aquifer and modeled ground-water flow with the U.S. Geological Survey's "Modular Three-Dimensional Finite-Difference Ground-Water Flow Model."

The hydrogeology and computer simulation of the Sundre aquifer in Ward and McHenry counties was prepared by Pusc (1987) in two parts. Part I contains basic ground-water data of the Sundre aquifer, including logs of test holes and wells, water levels in selected wells, stage height of the Souris River, discharge measurements of the Souris River, discharge measurements of Minot city wells and chemical analyses. Part II includes a discussion of the hydrogeology of the Sundre aquifer and a computer simulation of ground-water flow utilizing the U.S.G.S. "Modular Three-Dimensional Finite-Difference Ground-Water Flow Model."

CHAPTER III

HYDROGEOLOGIC SETTING

Surficial Geology

The surficial geologic materials that underlie the study area consist of Pleistocene glaciofluvial and Holocene alluvial deposits. These surficial deposits can be divided into two major stratigraphic units: the Oahe Formation and the Coleharbor Group (Clayton and others, 1980).

The Coleharbor Group consists of Pleistocene glacial deposits in the study area. As the result of at least three major glacial events, drift was deposited in thicknesses exceeding 500 feet in some places, but in the study area the average is 100 feet (Pettyjohn and Hutchinson, 1971). The drift consists mainly of ground moraine, end moraine, outwash, ice-contact deposits and glacial lake deposits.

The most common surficial material in the Minot area is ground moraine, which is composed of clay, silt, sand, gravel and boulders, in which clay and silt predominate (Pettyjohn, 1967A). Pebbles and larger clast are generally carbonate rocks, with minor granitic and gneissic rocks (Lemke, 1960).

Outwash deposits are of importance in local areas, where they can reach a thickness of 150 feet (Pettyjohn and Hutchinson, 1971). The outwash is composed mainly of sand and gravel, and occurs predominantly in major river valleys. Large quantities of water can be stored and produced from these sediments, as demonstrated by the Minot well field.

The Oahe Formation is composed of unconsolidated sediments deposited from the end of the last glaciation (10,000 years B.P.) to the present. The majority of these deposits lie within the floodplains of the Souris River and its major tributaries and consist of alluvial sediments (clay, silt, sand and gravel). These deposits have a complex depositional history as a result of the Souris River changing course several times (Pusc, 1987B).

Sundre Aquifer

The Sundre aquifer (formerly termed the Northwest Buried Channel aquifer, South Hill aquifer and Sundre Buried Channel aquifer, Pettyjohn, 1970) lies within a bedrock valley near Minot. Figures 3 and 4 show the location and orientation of the bedrock valley in North Dakota. This buried bedrock valley has been traced across North Dakota for over 100 Miles (Lindvig and Schmid, 1982).

The aquifer ranges from 1 to 2 miles in width and 30 to 250 feet in thickness (Pusc, 1987B). The thickest portion occurs in the area where the Souris River valley overlies the aquifer.

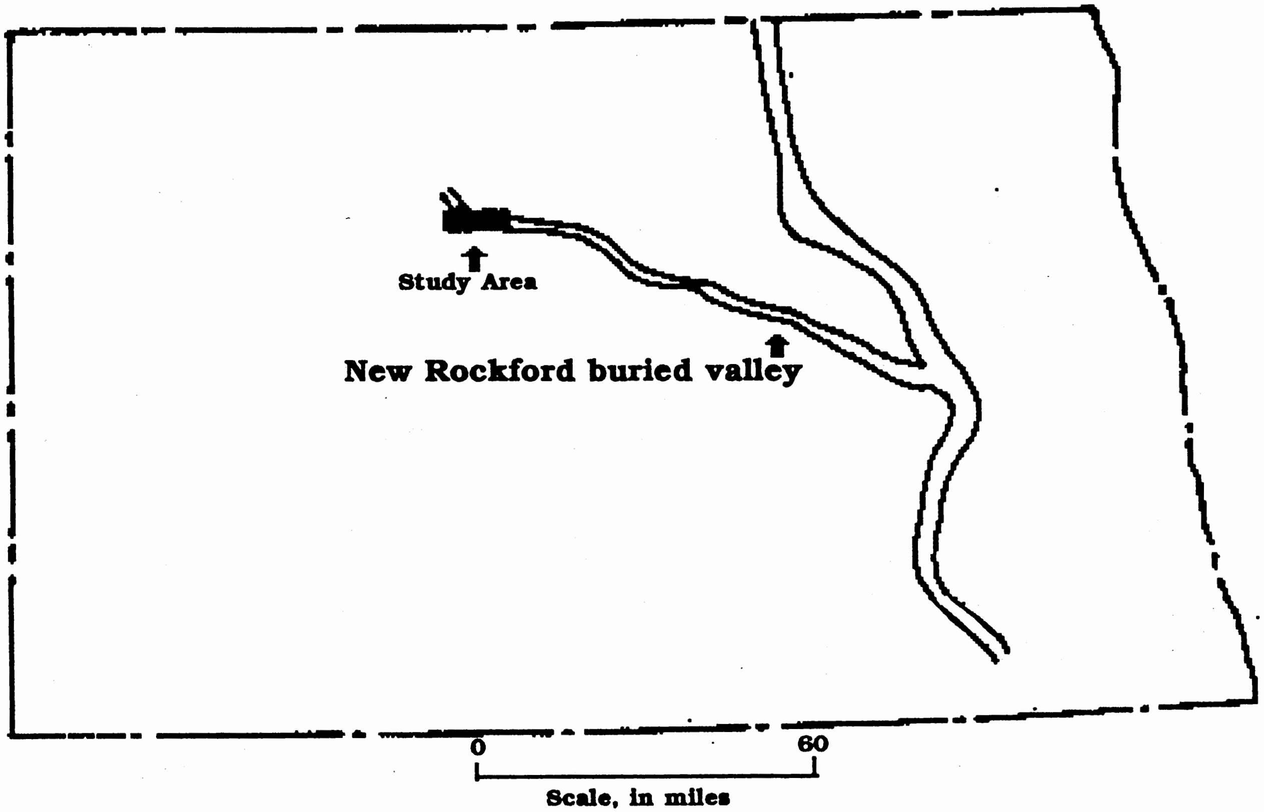


Figure 3. Location of study area and trend of New Rockford buried valley in North Dakota (modified from Kehew, 1986)

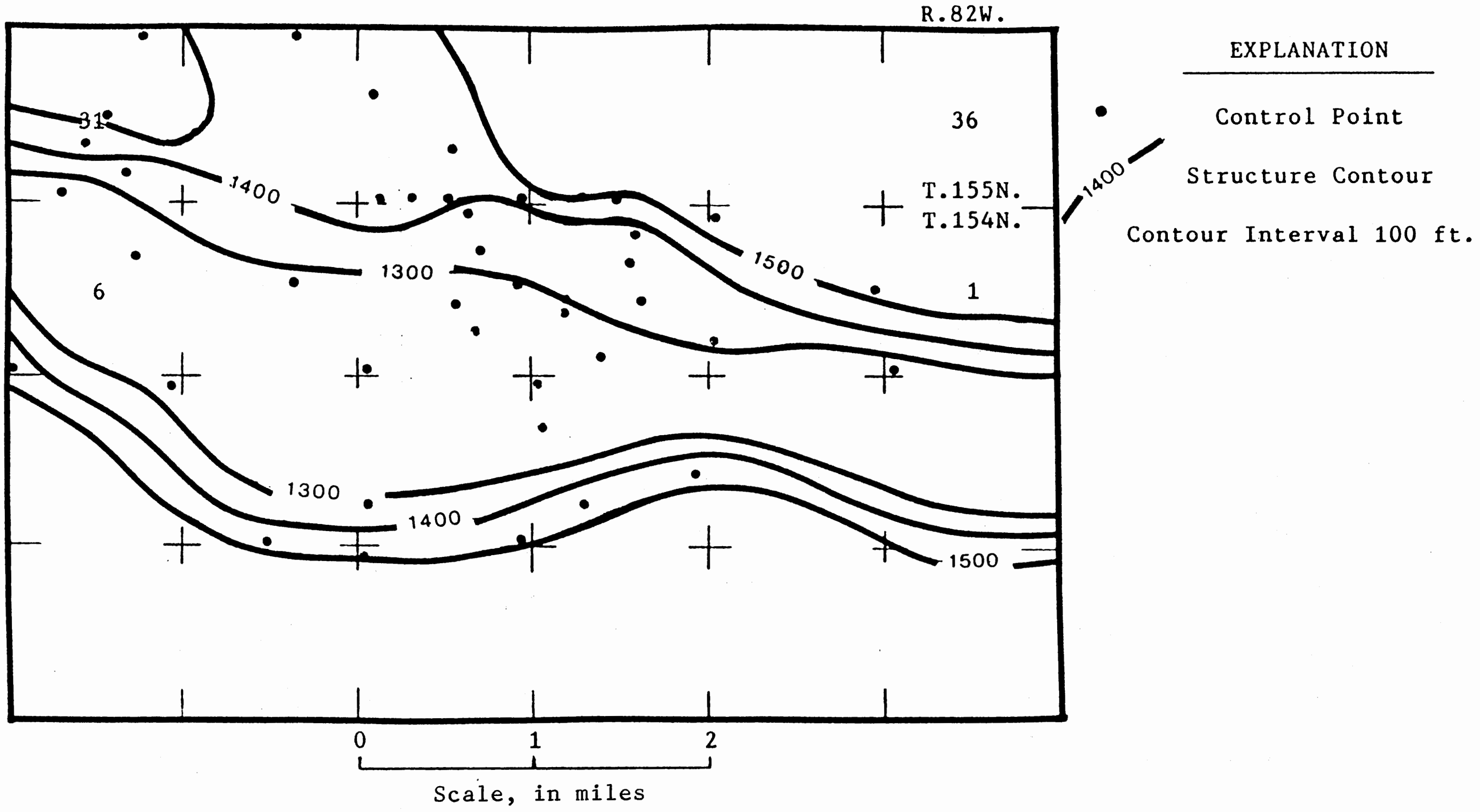


Figure 4. Bedrock Surface Map

The Sundre aquifer, part of the Coleharbor Group, is composed mainly of sand and gravel, with interbeds of silt and clay. The sand and gravel is composed mainly of silicates, carbonates, shales and lignite, derived from the Canadian Shield (Pusc, 1987B). The coarsest gravels are reported to lie along the axis of the buried valley (Pusc, 1987B). Isopach maps of the gravel and coarse sand indicate thickening toward the axis of the valley (Poore, 1987). Figure 5 shows the location of production and observation wells, and cross-sections used in this study. Stratigraphic cross-sections of the Sundre aquifer are included as figures 6 and 7.

The Lower Souris aquifer averages 90 feet in thickness where it overlies the Sundre aquifer. To the east and west of the Souris River valley, the Sundre aquifer is overlain by 15 to 50 feet of fluvial silt and clay and up to 200 feet of glacial till.

Low transmissivity barriers isolate the Sundre aquifer from eastern and western extensions of the buried valley aquifer system. The western barrier is located just southeast of Minot, with the eastern barrier east of the study area in McHenry county. The length of the buried valley within the low transmissivity barriers is reported to be 18 miles long (Pusc, 1987B).

Lower Souris Aquifer

The Lower Souris aquifer is defined as all coarser

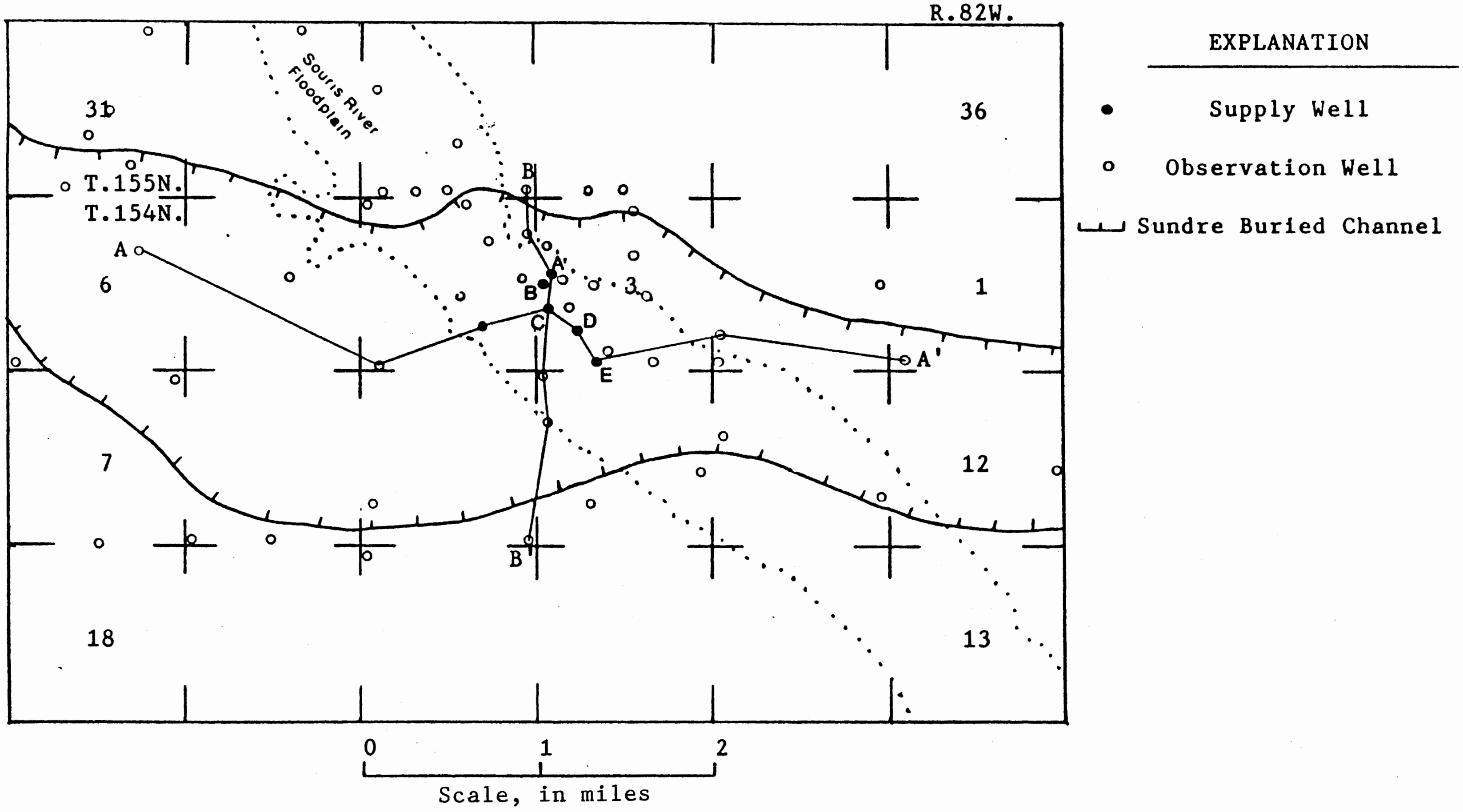


Figure 5. Well and Cross-Section Location Map

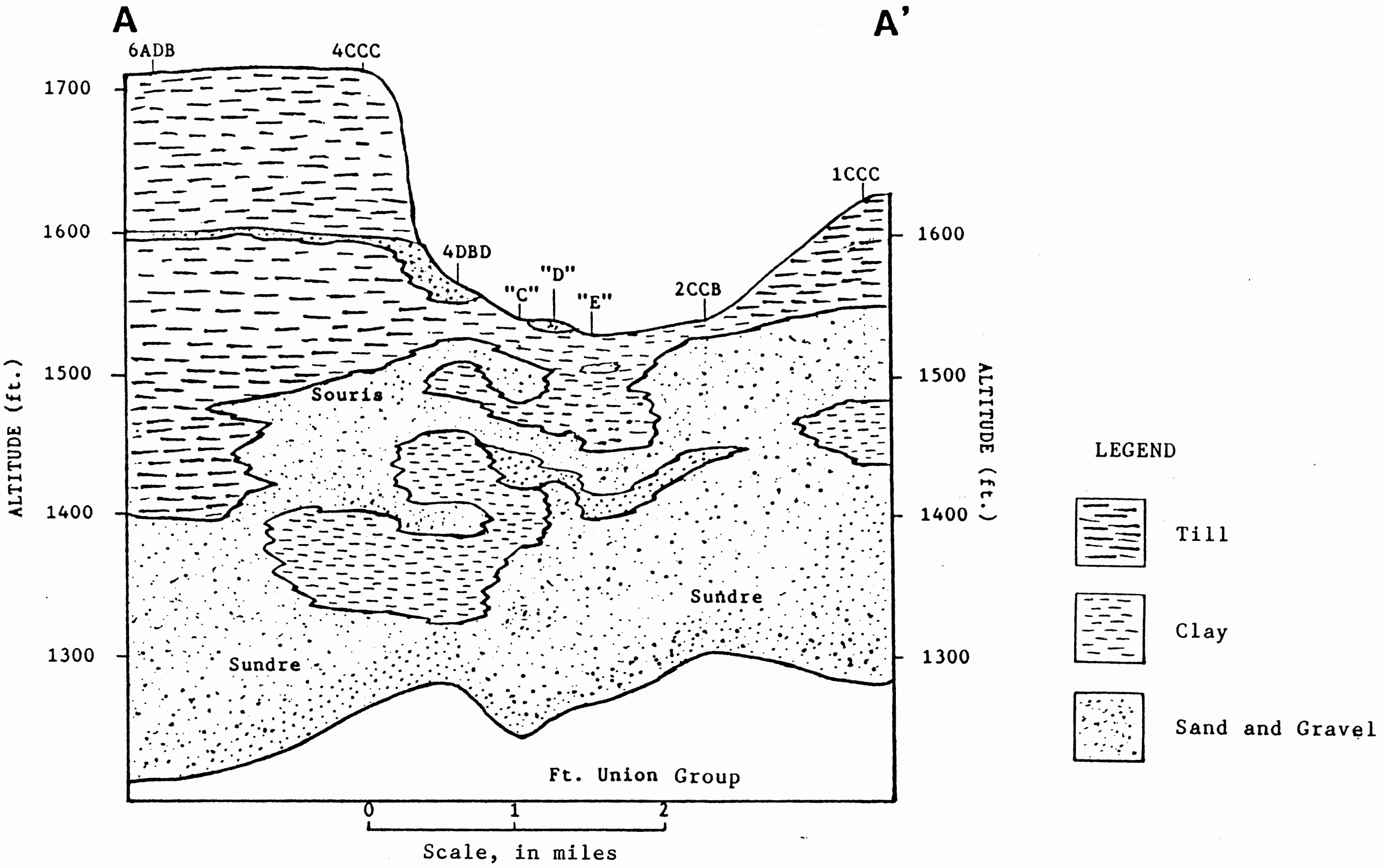


Figure 6. Stratigraphic Cross-Section A-A'

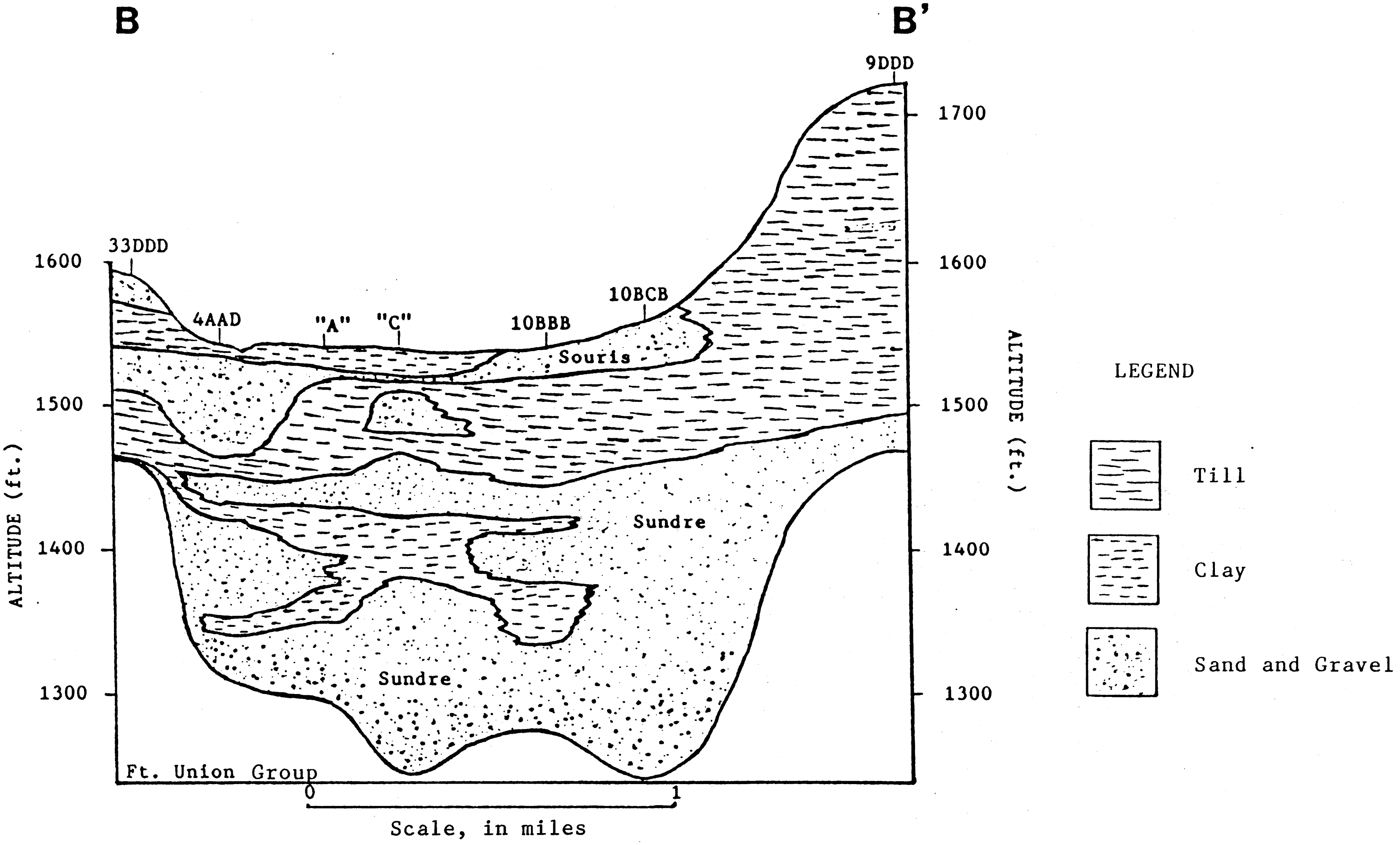


Figure 7. Stratigraphic Cross-Section B-B'

grained sediments (i.e. sand and gravel) of the Oahe Formation located within the Souris River valley southeast of Minot, within the study area (figure 5). Sand and gravel intervals usually range from 5 to 90 feet. The water table is commonly 5 feet or less below land surface (Pusc, 1987B). The importance of the Lower Souris aquifer to this investigation, is the hydraulic connection which it provides between the overlying Souris River and the underlying Sundre aquifer. The Souris aquifer is the source of substantial recharge to the Sundre aquifer (Poore, 1987).

Bedrock Geology

The Fort Union Group, of Tertiary age, unconformably underlies the Coleharbor Group in the study area. The four formations which compose the Fort Union Group are, in ascending order, the Ludlow, Cannonball, Tongue River and Sentinel Butte. The Ludlow Formation is composed of interbedded shale, siltstone, sandstone, bentonitic claystone and lesser amounts of lignite. The Cannonball Formation is composed of dark-gray sand, clay and a few thin beds of nodular, fossiliferous limestone and is of marine origin (Pettyjohn and Hutchinson, 1971). The highest chloride concentrations in the study area are usually associated with the Cannonball. The Tongue River Formation, which crops out along the Souris River valley, is a continental deposit of clay, silt, sandstone and numerous lignite beds (Pettyjohn and Hutchinson, 1971). A sodium bicarbonate type water is usually reported with the Tongue River Formation. The Sentinel Butte is lithologically similar to the Tongue River and is undifferentiated.

The individual formations of the Fort Union Group are undifferentiated in the field and are treated as one bedrock unit for the purposes of this investigation. The unconformable surface of the Fort Union dips in a northeasterly direction and the Group as a whole, thickens in a westerly direction.

Wells capable of flowing are reported in the Fort Union Group. A combination of considerable amounts of dissolved gas in the water as well as artesian conditions are reported by Pettyjohn (1970). Most wells completed within the bedrock yield only small quantities of water. Wells which tap layers of lignite may produce brown or even black water as a result of finely divided lignite and organic acids in the water (Pettyjohn, 1970).

CHAPTER IV

HYDROGEOCHEMISTRY

Introduction

The hydrogeochemistry of the Sundre aquifer was evaluated to develop a geochemical model to facilitate the implementation of the solute-transport model. To understand the Sundre aquifer, it is necessary to investigate the hydrogeochemistry of the deposits which supply recharge to the Sundre aquifer. The geochemical model should explain the occurrence of the major ions present in the ground water, as well as possible sources and sinks for these ions. The ground water is predominantly a sodium bicarbonate sulfate type, with a calcium sulfate type present in shallow horizons. Sulfate is the ion of most concern to this study, as it is present in Minot Municipal well E at concentrations of 1,000 mg/l, four times the recommended level of 250 mg/l (U.S. Public Health Service, 1962). Sulfate concentrations as high as several thousand mg/l have been reported in shallow till horizons by Pettyjohn, (1968).

Geochemical Model

The geochemical model must account for the presence of sulfate levels of several thousand mg/l, sodium concentrations of several hundred mg/l and bicarbonate levels in excess of 700 mg/l. Calcium concentrations are usually less than 300 mg/l, with magnesium levels normally less than 100 mg/l. The chloride ion concentration rarely exceeds 100 mg/l. Other ions present occur only in small concentrations and do not influence the most important chemical reactions taking place.

The pattern of annual precipitation in the study area is important to the geochemical model. The average annual precipitation is 16-17 inches, half of which comes during May-July (Pettyjohn, 1967A). The precipitation during the summer months is in the form of convective thunderstorms. These storms produce large quantities of rainfall in short time periods.

The geochemical process begins with the infiltration of rain and snowmelt into the ground surface, where it becomes charged with CO_2 in the organic rich horizons in the upper part of the soil profile. The addition of CO_2 decreases the pH of the water. The increased acidity of the water acts to dissolve carbonate minerals and liberates calcium, magnesium and bicarbonate ions. The dissolution of calcite can be expected to take place at a faster rate than the dissolution of dolomite, resulting in a substantially higher concentration of calcium than magnesium.

$$2CH_2O \rightleftharpoons CO_2 + CH_4$$

$$CaCO_3 + CO_2 + H_2O \rightleftharpoons Ca^{++} + 2HCO_3^-$$

$$CaMg(CO_3)_2 + 2CO_2 + 2H_2O \rightleftharpoons Ca^{++} + Mg^{++} + 4HCO_3^-$$

Two hypotheses for the high sulfate concentrations are (1) erosion and incorporation of sulfate-rich bedrock minerals into the glacial deposits, and (2) oxidation of reduced forms of sulfur, which were incorporated into the till during glaciation. The till which mantles the bedrock in the study area can be divided into two distinct zones, (1) a yellow-brown oxidized horizon ranging from 20 to 40 feet thick and (2) a gray unoxidized till which underlies the oxidized horizon. The highest sulfate concentrations in the study area have been reported in the shallow oxidized till horizons (Pettyjohn, 1968). The association of the highest sulfate concentrations with the oxidizing environment suggest that oxidation of sulfides is occurring in the study area.

Examination of over 200 sample logs of test holes drilled in Ward and Renville counties failed to reveal any indication of sulfate-rich minerals or inorganic sulfides, such as pyrite or marcasite (Pettyjohn, 1968). No petrographic data were available for the immediate study area. Petrographic examinations conducted south of the study area revealed gypsum precipitated in place (Groenewold, 1983). A subsequent study of tills in southern Canada also interpreted gypsum to be authigenic (Hendry and others, 1986). Both of these studies reported the presence of gypsum only in the shallow oxidized zone. The fact that the gypsum was precipitated in place, under oxidizing conditions suggest the oxidation of sulfides as the source of sulfate.

Examination of sample logs of test holes drilled in Ward and Renville counties revealed an abundance of lignite (Pettyjohn, 1968). A report on the geology of the Souris River area by Lemke, (1960) also describes lignite present in the bedrock as seams up to 15 feet thick and disseminated throughout the glaciofluvial deposits which mantle the bedrock. The lignite provides an abundant source of organic sulfide. Using geochemical and isotopic data, Hendry (1986) found that in southern Canada, organic sulfides present as lignite are the principal source of sulfate.

The oxidation of organic sulfides releases hydrogen ions, which reduces the pH of the pore water and dissolves carbonate minerals present. The abundance of sulfate and calcium results in the precipitation of gypsum if over-saturation occurs due to evapotranspiration.

$$2S + 3O_2 + 2H_2O \rightleftharpoons 2SO_4^{--} + 4H^+$$

$$CaCO_3 + H^+ \rightleftharpoons Ca^{++} + HCO_3^-$$

$$CaMg(CO_3)_2 + 2H^+ \rightleftharpoons Ca^{++} + Mg^{++} + 2HCO_3^-$$

$$Ca^{++} + SO_4^{--} + 2H_2O \rightleftharpoons CaSO_4 + 2H_2O$$

The abundance of Na-montmorillonite clays, which act to facilitate ion exchange provides a source for the sodium concentrations observed (Kehew, 1983). Evaporation as a source for sodium was rejected, as chloride concentrations are not high enough to explain the sodium concentrations present without an additional source of sodium. Calcium and to a lesser extent magnesium are adsorbed on the exchange sites on the clay particles, while sodium is liberated into solution. The removal of calcium ions facilitates the further dissolution of carbonate minerals. This process may continue until saturation of sodium occurs. Sodium sulfate (Glauber salt) occurs as brine in lake water and in beds at the bottom of some lakes west of the study area (Lemke, 1960). Figure 8 shows a increase in the Na : Ca ratio as depth increases. This suggest that the exchange process continues as the water infiltrates downward.

$$Ca^{++} + 2NaX \rightleftharpoons 2Na^{+} + CaX_2$$

$$Mg^{++} + 2NaX \rightleftharpoons 2Na^{+} + MgX_2$$

A computer program (WATEQF) developed by Plummer and others (1976) was used to calculate the saturation indices for gypsum, calcite and dolomite. The indices were evaluated for waters representing increasing depth and are plotted in figure 9. No sample data were available for the unsaturated zone, where equilibrium conditions for gypsum might be expected. Figure 9 shows a decreasing saturation index for each mineral with increasing depth. Gypsum is near equilibrium in the shallow oxidized zone and rapidly becomes undersaturated with an increase in depth, as would be expected if its source were in the shallow horizons where oxidizing conditions are present.

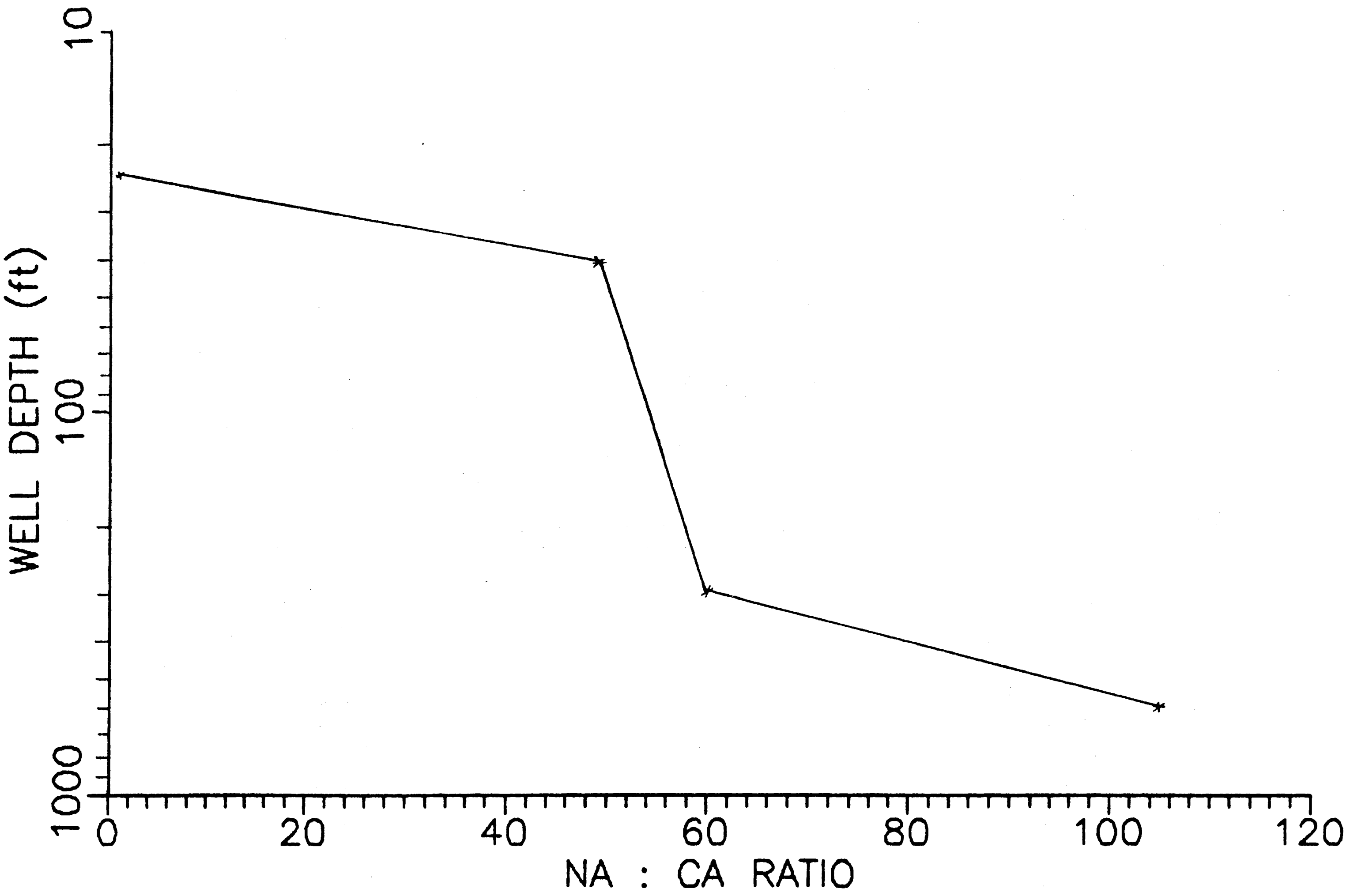


Figure 8. Na:Ca Ratio Versus Depth

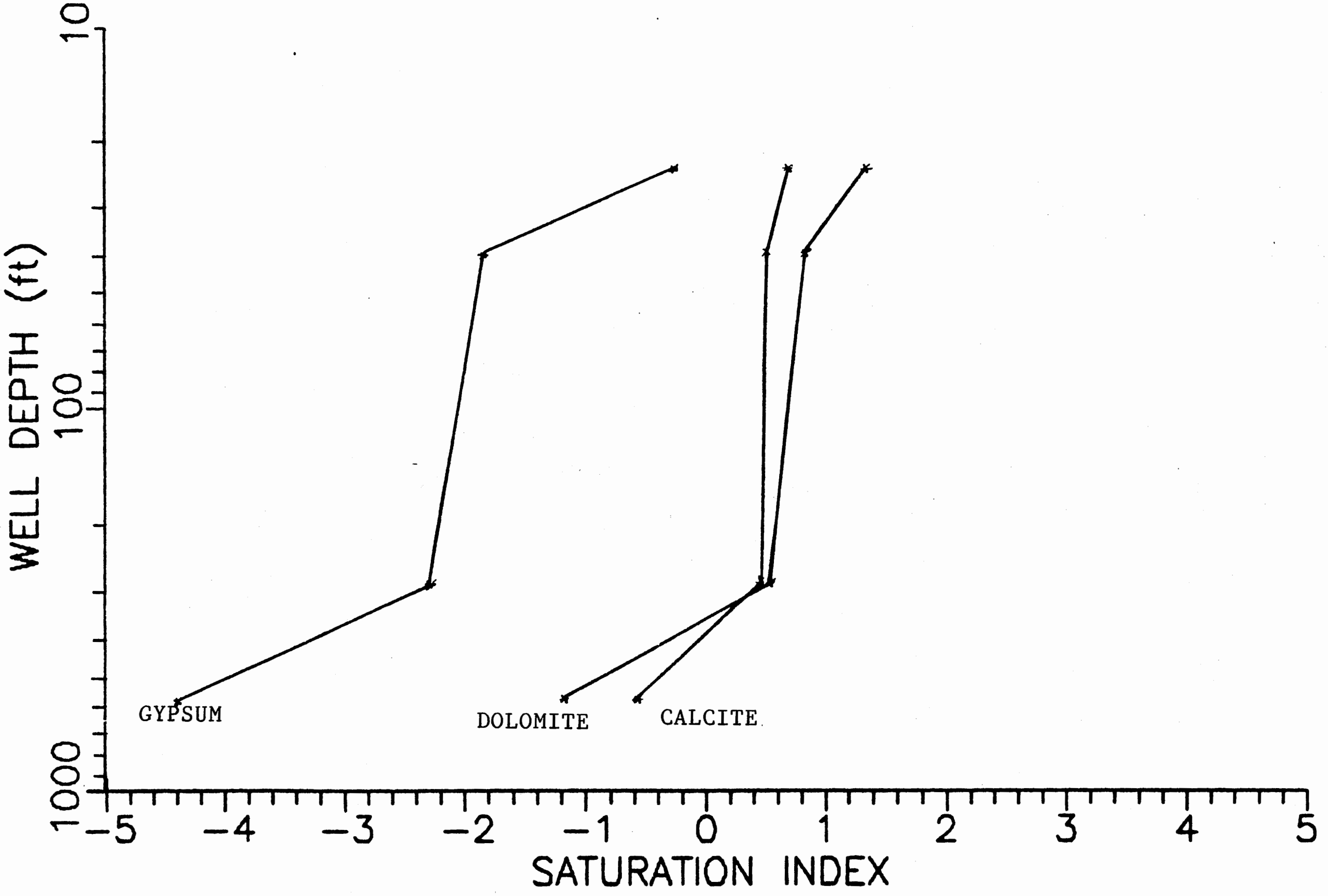


Figure 9. Saturation Index Versus Depth

The majority of the chemical processes determining the water quality appear to be operating only in the unsaturated zone. Ion exchange is the exception in that, it will continue to act as the water infiltrates through the saturated zone. Calcium sulfate type waters occurring at shallow depths change to sodium sulfate waters at greater depths (Pettyjohn, 1968). The evidence which suggests that the oxidizing environment plays the major role in the geochemical evolution of the ground water, also supports the hypothesis that sulfate is the result of oxidation of organic sulfides. Minor amounts of sulfate may be the result of dissolution of sulfate-rich minerals incorporated in the sediments during glaciation.

A schematic diagram of the chemical processes and salt movement appears as figure 10. The majority of rainfall events do not provide sufficient quantities to result in ground-water recharge, but only serve to concentrate salts in the shallow horizons. Exceptional rainfall events during the summer months flush the accumulated salts down to the ground water (Moran and others, 1978).

Ground-Water Mixing Evaluation

The geochemical model presented above details the processes controlling the evolution of ions in the ground water, but does not totally explain the hydrogeochemistry of the Sundre aquifer in the study area. Chemical analyses from the five municipal supply wells completed in the Sundre

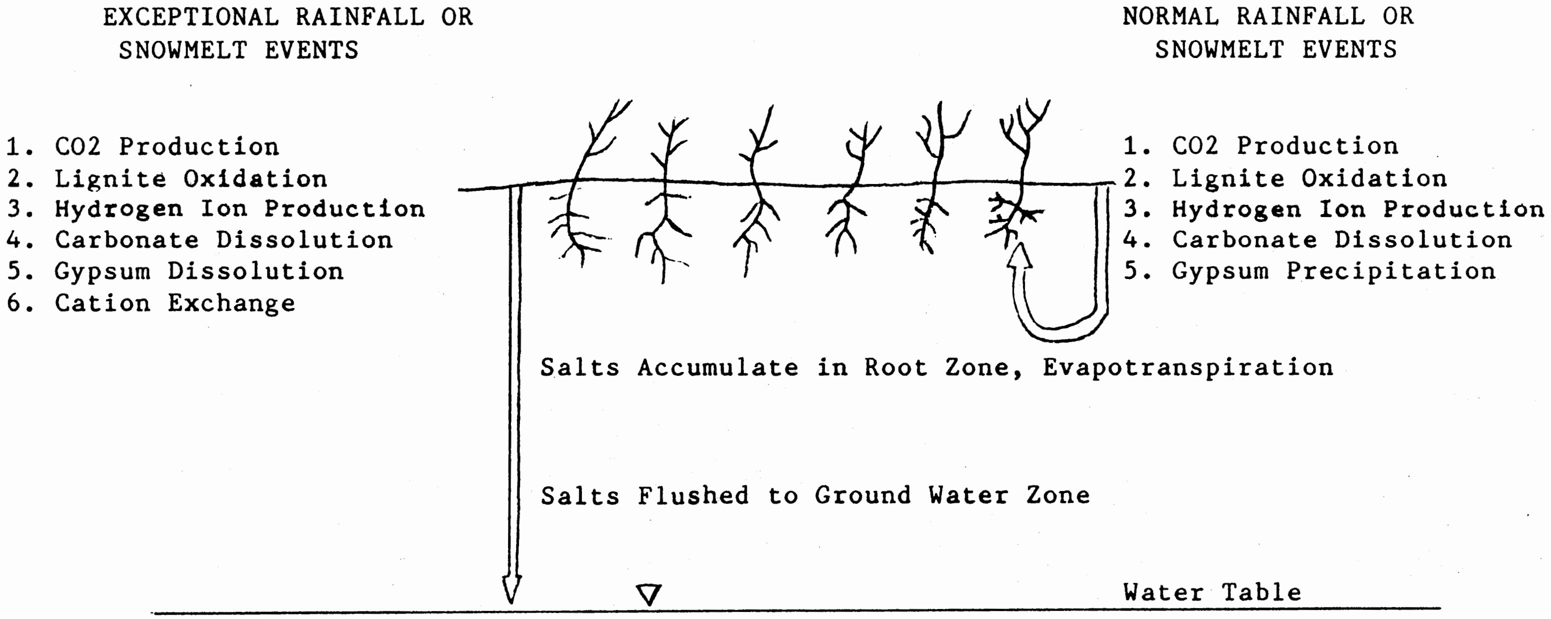
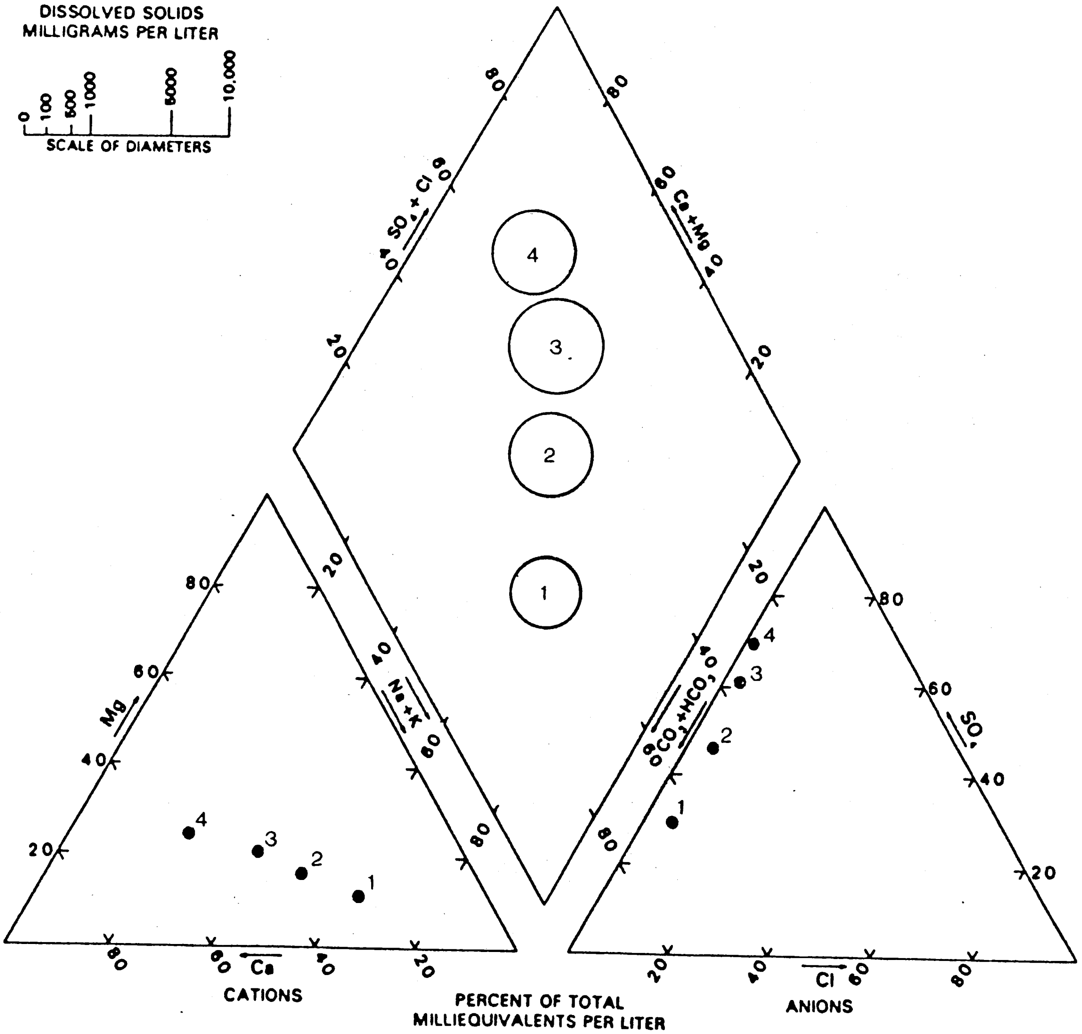


Figure 10. Schematic Diagram of Chemical Processes and Salt Movement (modified after Moran et al, 1978)

aquifer indicate large water quality changes within short distances. Plots of the major ions' concentrations over time are provided for each well in Appendix A. Wells D and E show substantial increases in the dissolved ion concentrations over time. Wells A, B, and C tend to remain unchanged over the time period analyzed. The total dissolved solids were calculated for each well, with wells A, B and C having similar TDS. Well D showed an increase, with well E having the highest TDS. These results suggest possible mixing of waters within the Sundre aquifer.

A computer program (WATEVALG) written by Hounslow and Goff (1989) to evaluate the mixing of waters was used to check this hypothesis. Four analyses were chosen to assess the mixing scenario. The analysis of well A was chosen as one end-member, to represent the fresher waters derived through leakage from the overlying Souris aquifer. The other end-member selected was an analysis from a shallow till horizon located at 154-082-12DAA4, to the east of the well field, which represents the present source area for high sulfate concentrations. Piezometric maps (Appendix B) indicate the regional up-gradient direction to lie east of the well field. Two analyses were chosen, which lie along the ground-water flow path between the two end-members. These analyses were from well D and multiple piezometer location 154-082-12DAA1, screened in the Sundre aquifer.

Figure 11 is a representation of the Piper plot produced by the program, on which the four previously



1. Well A, Sundre aquifer
2. Well D, Sundre aquifer
3. 154-082-12DAA1, Sundre aquifer
4. 154-082-12DAA4, Shallow Till Horizon

Figure 11. Piper Plot Mixing Evaluation

described analyses are plotted. The four analyses plot on relatively straight lines on both the anion and cation plots, indicating a simple mixing of waters from well A and the till horizon to produce the two intermediate compositions.

BALANCE, a computer program used to determine the quantities of minerals or phases entering or leaving the aqueous phase was also used to evaluate mixing of waters (Parkhurst and others, 1982). The BALANCE investigation was used to study mixing within the Sundre well field, between well A, to the north, and well E to the south. The results of the mixing of waters from well A and well E are presented in Table I. The mix, which represents well D is shown to consist of 50% well A and 50% well E. Negative values for the "delta Phases" indicate precipitation, while positive values indicate dissolution. The quantities are reported in mmol/l. The most active processes are the precipitation of gypsum and cation exchange. The mixing of waters appears to be occurring as evidenced from both the Piper plot and the Balance program.

The water quality at well E is indicative of the water quality away from the area receiving seepage from the overlying Souris aquifer. The sulfate concentration was shown to increase away from the intersection of the Sundre and Souris aquifers in a previous study by Pettyjohn (1970).

The degradation of the water quality in wells D and E from 1975, the time of initial pumping, to 1986 is the

TABLE I

"BALANCE" MIXING RESULTS

"D" FINAL		"A" INIT1	"E" INIT2	CALCITE	DOLOMITE	GYPSUM	HALITE	CO2 GAS	ION EXCH
3.240	CA	1.820	5.740	1.000	1.000	1.000	.000	.000	-1.000
1.650	MG	.860	2.470	.000	1.000	.000	.000	.000	.000
8.700	NA	8.260	15.220	.000	.000	.000	1.000	.000	2.000
.200	K	.100	.300	.000	.000	.000	.000	.000	.000
4.160	S	1.980	9.790	.000	.000	1.000	.000	.000	.000
1.470	CL	.870	1.330	.000	.000	.000	1.000	.000	.000
9.300	C	8.750	11.590	1.000	2.000	.000	.000	1.000	.000
1.000	MIX	1.000	1.000	.000	.000	.000	.000	.000	.000

DELTA PHASES

INIT1	.5000
INIT2	.5000
CALCITE	-.5050
DOLOMITE	-.0150
GYPSUM	-1.7250
HALITE	.3700
CO2 GAS	-.3350
ION EXCH	-1.7050

result of ground-water flow reversals. This change in ground-water flow direction is exhibited in the series of piezometric level maps for the Sundre aquifer included as Appendix B. Under predevelopment conditions, seepage from the Souris aquifer entered the Sundre aquifer in the vicinity of wells A, B, and C, and flowed south toward wells D and E, resulting in mixing with the connate water in the Sundre aquifer. With the reversal in flow direction as the result of pumping from the well field, less of the fresher water from the overlying Souris aquifer reached wells D and E. The sulfate levels in wells D and E increased as water with a higher sulfate concentration was drawn towards the cone of depression created by the well field.

Further evidence for the mixing of waters can be shown from the affect of the pumping rate of well D on the water quality of wells D and E. Figure 12 displays the pumping rates of wells D and E versus time and the sulfate concentrations of wells D and E versus time. The figure shows the substantially smaller pump rate of well E, when compared to well D. It is for this reason that the pump rate of well D is considered the most important of the two wells. The graph indicates that each time the pump rate of well D is reduced substantially, the sulfate concentration decreases in well E and increases in well D.

Figures 13 and 14 are plots of the pump rate of well D versus the sulfate level in well D and in well E, respec tively. Correlation coefficients were calculated for each

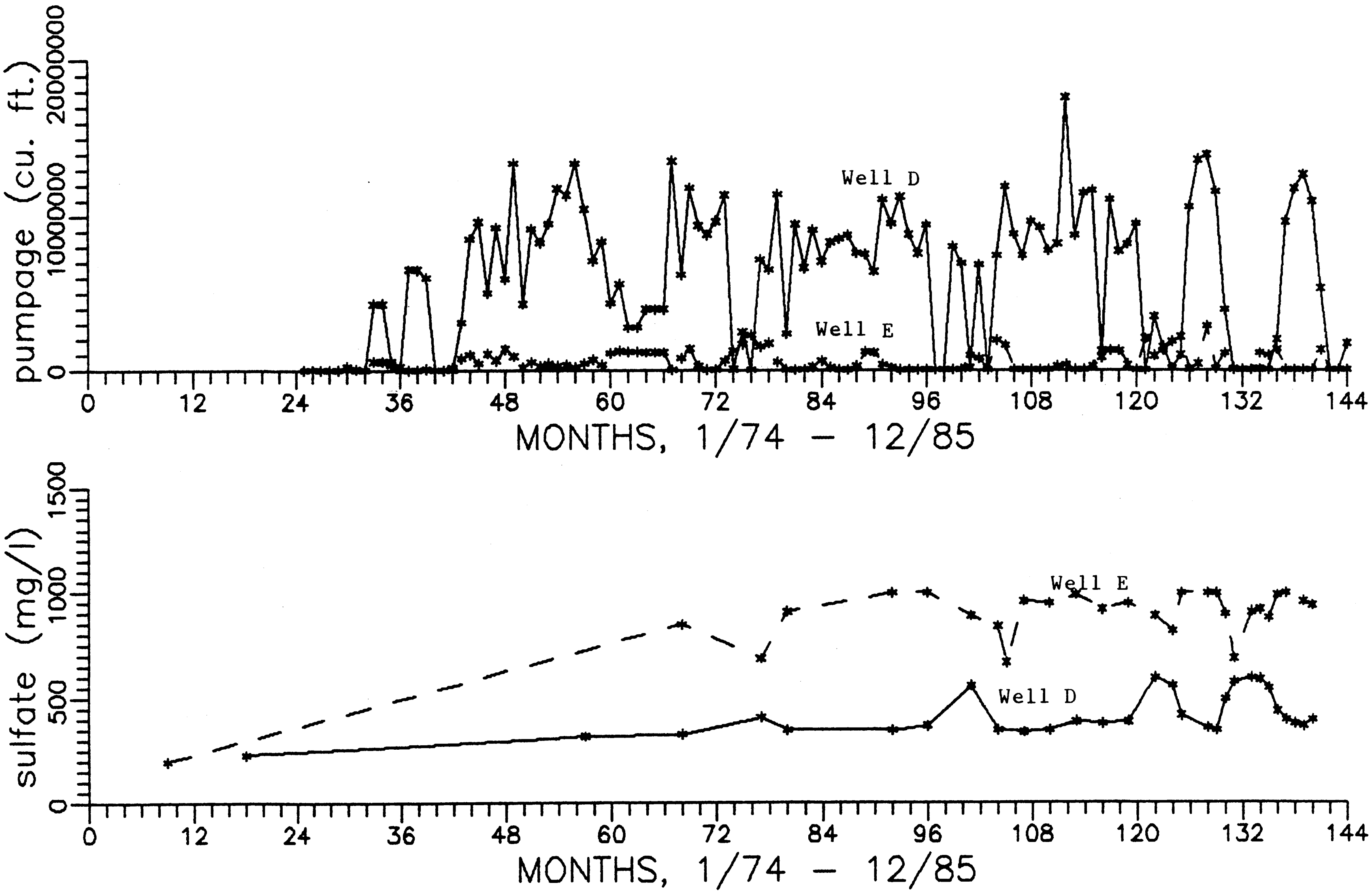


Figure 12. Pump Rates in Wells D and E versus Sulfate Concentrations in Wells D and E

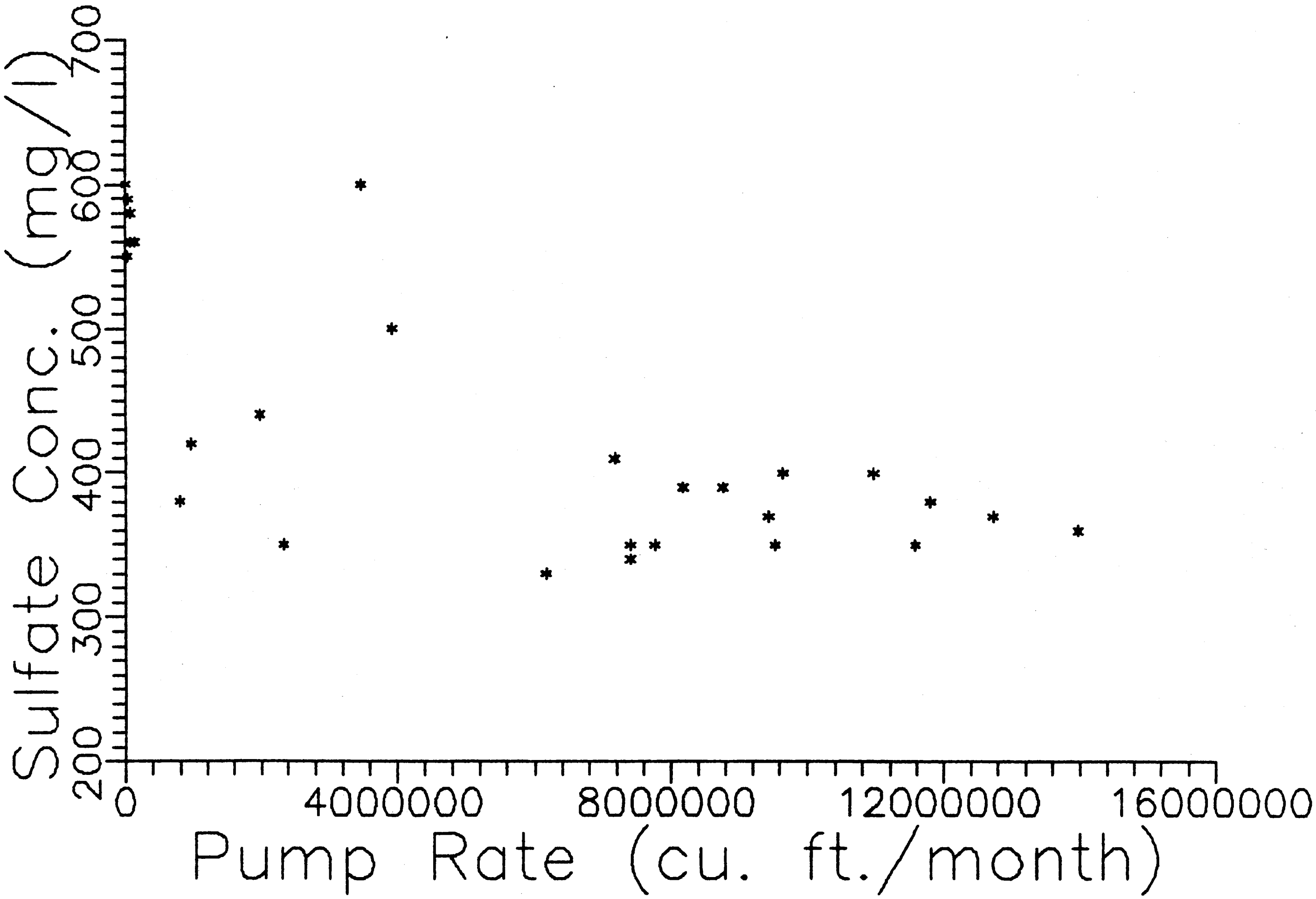


Figure 13. Pump Rate for Well D Versus Sulfate Concentration in Well D

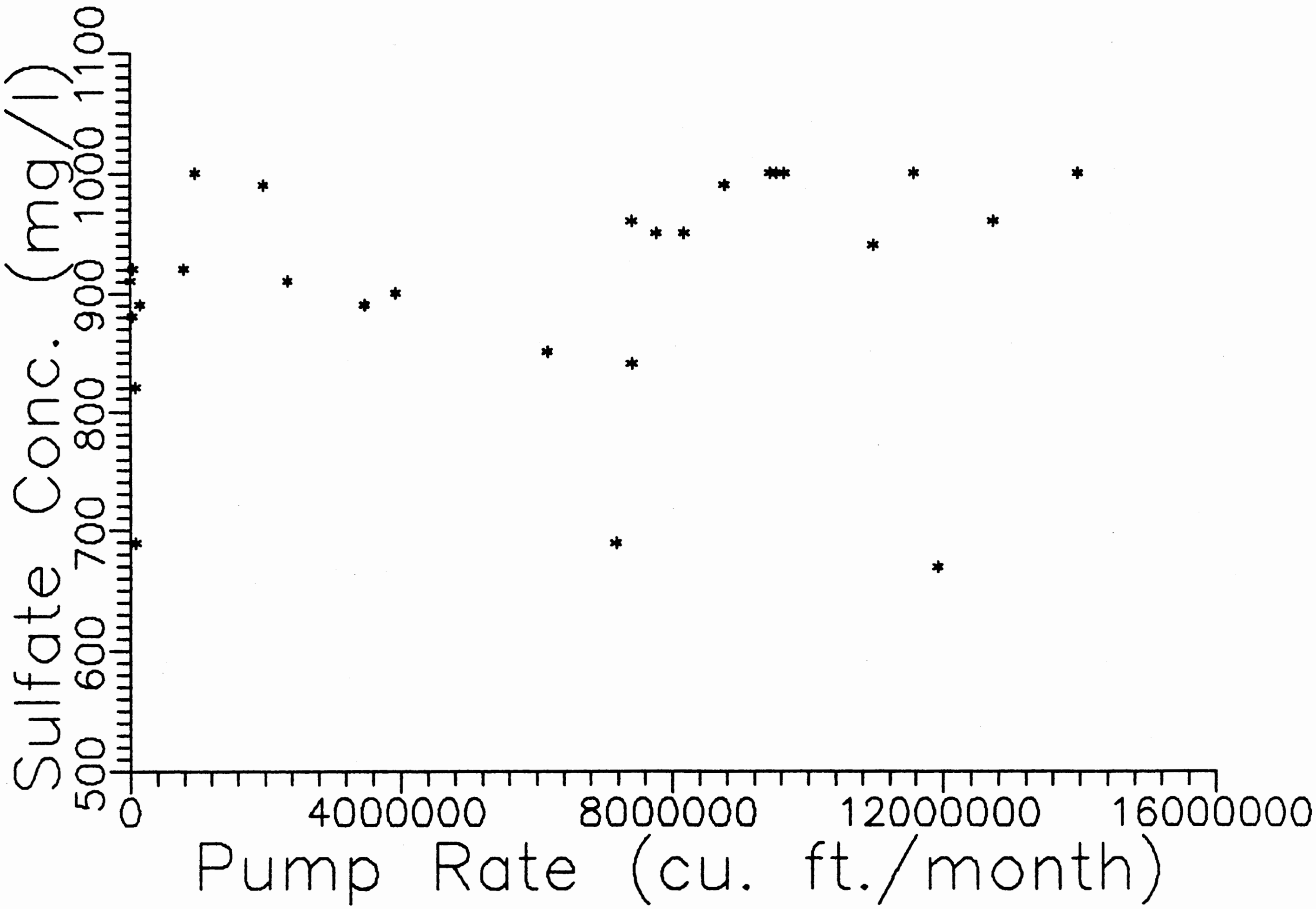


Figure 14. Pump Rate for Well D Versus Sulfate Concentration in Well E

set of data, and indicate that in well D there is a negative correlation, with approximately 50% of the variation of pumping rate and sulfate concentration explained by the association of the two variables. The correlation coefficient for the sulfate level in well E and the pump rate of well D does not indicate that the two variables are associated.

The improvement in the quality of the water in well E when well D reduces its pumping rate, is explained as follows. While well D is pumping, it intercepts the fresher waters to the north and prevents them from mixing with the poorer quality waters to the south, which would act to lower the sulfate concentrations in well E (figure 15). Conversely, when well D does not capture the waters from the north, mixing takes place and results in the recorded improvement in well E. The sulfate concentration increases in well D when its pump rate is reduced, due to less water being drawn from the north to mix with the higher concentration waters in the vicinity of well D. When well D is pumping at a high rate, it is capable of pulling water from the north to mix with the poorer quality water located to the south.

The geochemical data indicate that the sulfate concentrations in the Sundre aquifer are the result of the oxidation of organic sulfides present within the till. Henry (1986) reported that the hydraulic conductivity of weathered and nonweathered till, in western Canada averages

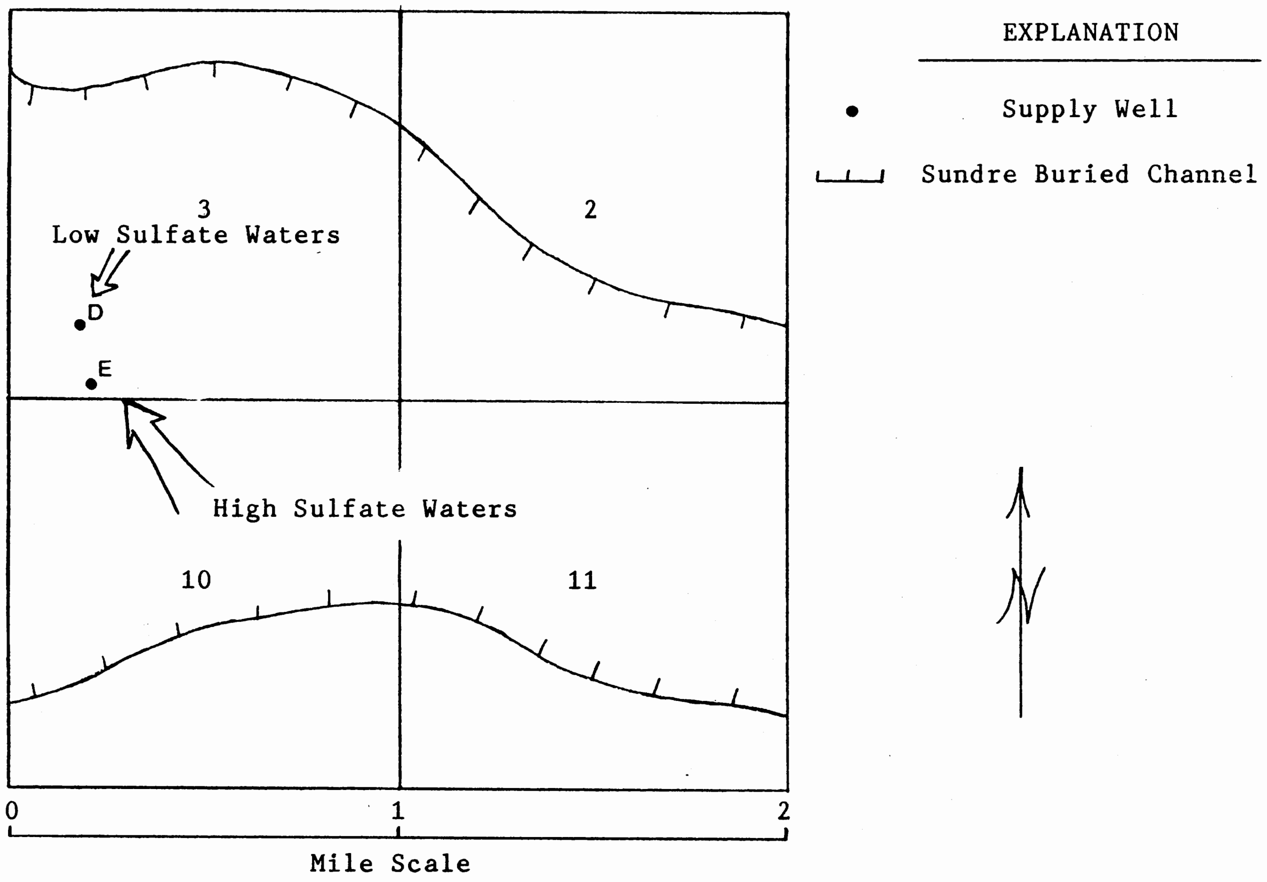


Figure 15. Sulfate Concentration Relative to Wells D and E

about $4.5 * 10^{-6}$ and $2.2 * 10^{-10}$ gpd/ft sq, respectively. These low hydraulic conductivity values indicate that the present surficial oxidizing horizon likely could not have contributed significant quantities of sulfate to the Sundre aquifer, which lies approximately 200 feet beneath the oxidized till horizon.

A comprehensive study of the till in South Dakota by Cravens and Ruedisili (1987) indicated that recharge through the till to underlying outwash deposits is insignificant. The age of the water in the buried outwash deposits was determined to be in excess of 9,000 years old.

Pettyjohn (1967B) reported the presence of multiple oxidized zones within the glacial drift and at the top of the Fort Union Group, in the Minot area. These oxidized zones were formed on the surface of deposits of till emplaced during different advances and retreats of the glacier. The compositional similarity of all of the till deposits suggests that oxidation, regardless of age, should have resulted in similar chemical processes as those currently operating at the surface. It is suggested, that buried oxidized zones, representing older till deposits, may be both the source and in hydraulic connection with the high sulfate-containing segment of the Sundre aquifer. Consequently, buried oxidized zones are the cause of the high sulfate concentrations observed in parts of the Sundre aquifer.

CHAPTER V

HYDRAULIC CHARACTERISTICS

Introduction

The solute-transport model used in this study required the knowledge of several hydraulic characteristics of the aquifer. These characteristics are as listed: transmissivity, hydraulic conductivity, longitudinal dispersivity, transverse dispersivity, effective porosity, storativity and regional flow velocities in the X and Y directions. Most of these properties were determined from drill cutting samples and aquifer-tests as reported by previous authors.

Transmissivity

An aquifer test in the Sundre aquifer was conducted by Pettyjohn (1970), in which a well was drilled to a depth of 220 feet specifically for the test. The well had a specific capacity of 48 gpm/ft after pumping at 1950 gpm for 24 hours. The test lasted for approximately 15 days and operated at a rate of 1950 gpm. Water levels were measured in 37 observation wells in addition to the pumped well and ranged from 150 feet to 8.5 miles from the pumped well.

The cone of depression spread for more than seven miles laterally along the trend of the Sundre aquifer. Observation wells in the overlying Lower Souris aquifer recorded drawdown, which indicates leakage between the two aquifers. An area of greater than 28 square miles was reported to have provided recharge during the test. The transmissivity exceeded 250,000 gpd/ft, with twice this value reported where the Souris River valley overlies the Sundre aquifer. Numerous recharge and discharge boundaries were encountered during the test, complicating the interpretation of the data. The transmissivity can be expected to range from 150,000 to 240,000 gpd/ft, and average 200,000 gpd/ft.

Hydraulic Conductivity

The hydraulic conductivity (K) can be determined by dividing the transmissivity (T) by the saturated thickness (b); $K = T/b$. The thickness of the Sundre aquifer ranges from 30 to 250 feet, with all observation wells indicating the entire thickness to be saturated. The cross sections shown as figures 6 and 7 display an average thickness of 100 feet. These values result in the hydraulic conductivity values ranging from 600 gpd/ft sq to 8000 gpd/ft sq. The hydraulic conductivity is expected to average 2000 gpd/ft sq.

Longitudinal and Transverse Dispersivity

Longitudinal and transverse dispersivity are properties of the permeable medium and they influence the transport of a solute by hydrodynamic dispersion. This process results from two basic processes, molecular diffusion and mechanical mixing. The heterogeneity of hydraulic conductivity causes variations in the ground-water velocity, which results in mixing (Mackay and others, 1985).

There currently is no method to confidently predict the magnitude of dispersion for a previously unstudied field situation. If no detailed studies exist for the given field site, longitudinal and transverse dispersivities should be estimated based on values from previous studies in similar hydrogeological systems. An investigation in a similar hydrogeological system resulted in values of 70 feet for the longitudinal dispersivity and 14 feet for the transverse dispersivity (Pinder, 1973). These values should provide a adequate starting point for the model and can be adjusted for this particular site through calibration of the model.

Effective Porosity

Porosity can be defined as the volume of the pore space or voids divided by the total volume. For evaluation with a solute-transport model, the effective porosity is the parameter required for input. The effective porosity is slightly less than the total porosity and represents the porosity which is active in the transmission of fluids. A small portion of the porosity may consist of dead end or noninterconnected pores and not contribute to the movement of fluids.

Porosities of 20 - 35% are reported as average for sand and gravel, mixed (Fetter, 1988). An initial estimate of 25% was chosen for the effective porosity in this study.

Storativity

The storativity can be defined as the volume of water that is absorbed or expelled from storage per unit surface area per unit change in head (Fetter, 1988). Aquifer test conducted in 1969 indicated storativities ranging from .0003 to .06 for the Sundre aquifer in the study area (Pettyjohn, 1970). The higher values were reported to represent areas adjacent to the Souris River floodplain. The best value to represent the storativity in the study area is .0003 (Pettyjohn, 1970).

Ground-Water Velocity

The regional ground-water flow direction is along the trend of the Sundre aquifer to the west-northwest. This requires the separation of the velocity into X and Y components for the solute-transport model. The velocity was first calculated without considering any directional components. The velocity calculated with the equation shown below ranged from .1 to 1.2 ft/day, depending on the values used for each variable as defined below.

$$v = K * I / n * 7.48 \text{ (gal/cu ft)} \qquad (1)$$

v = ground-water velocity (ft/day)
K = hydraulic conductivity (gpd/ft sq)
I = hydraulic gradient, dimensionless
n = effective porosity (percent)

The values used for hydraulic conductivity (K) ranged from 600 to 8000 gpd/ft sq. The regional hydraulic gradient (I) was determined from the piezometric maps presented in Appendix B to average 1.5 ft/mile. A value of .25 was used for the effective porosity.

A velocity of .5 ft/day was considered to be the most likely value. As the ground water flows predominantly in a westerly direction, the X velocity component was assigned a value of .5 ft/day. A velocity of .1 ft/day was considered adequate to account for the slight northerly component of flow and was used for the Y component of flow.

CHAPTER VI

COMPUTER SIMULATION

Explanation of the Solute-Transport Model

An analytical version of the "Random-Walk" solute-transport model was chosen to simulate the mixing of waters within the Sundre aquifer. The model can simulate one- or two-dimensional nonsteady/steady flow problems in homogeneous and isotropic aquifers. A homogeneous aquifer is described as having the same properties, such as porosity, hydraulic conductivity, and thickness at all locations. Isotropic aquifers have the same intrinsic permeability in all directions (Fetter, 1988).

The transport of a solute takes place by dispersive and advective processes. The advective part of the transport equation is based on a particle in a cell method, while the dispersive part is solved with a random-walk technique. Chemical reactions such as adsorption and ion-exchange are handled with the retardation coefficient term.

The model can be advanced in varying time steps as desired to allow modification of the model between time steps. Pumping and injection wells can be added to the simulation at the beginning of each time step or their rates changed as necessary. Particles may be added at each time step to simulate a continuous source. A more detailed discussion of the capabilities and limitations of the model is provided by the authors (Prickett and others, 1981).

Model Development

The development of the model began with an evaluation of the sulfate distribution within the aquifer prior to the development of the Sundre well field. A map showing the concentrations at the production wells and test holes is shown as figure 16. The samples in the production wells were taken during completion, while those in the test holes were taken on dates prior to development of the well field. This map provides further evidence for the mixing of waters from the overlying Souris aquifer and the Sundre aquifer. The map shows concentrations of sulfate considerably higher to the east, or up-gradient from the junction of the Sundre aquifer and the Souris River floodplain, in which lies the Lower Souris aquifer. Sulfate concentrations are lower in the Sundre aquifer to the west or down-gradient from the area of mixing. Figures 17-19 show the movement of high sulfate concentrations from the east, toward the well field and specifically toward well D, which has the greatest pump rate.

Prior to entering these concentrations into the model, a decision as to the cell size was made based on the method used to locate wells. The well-numbering system used

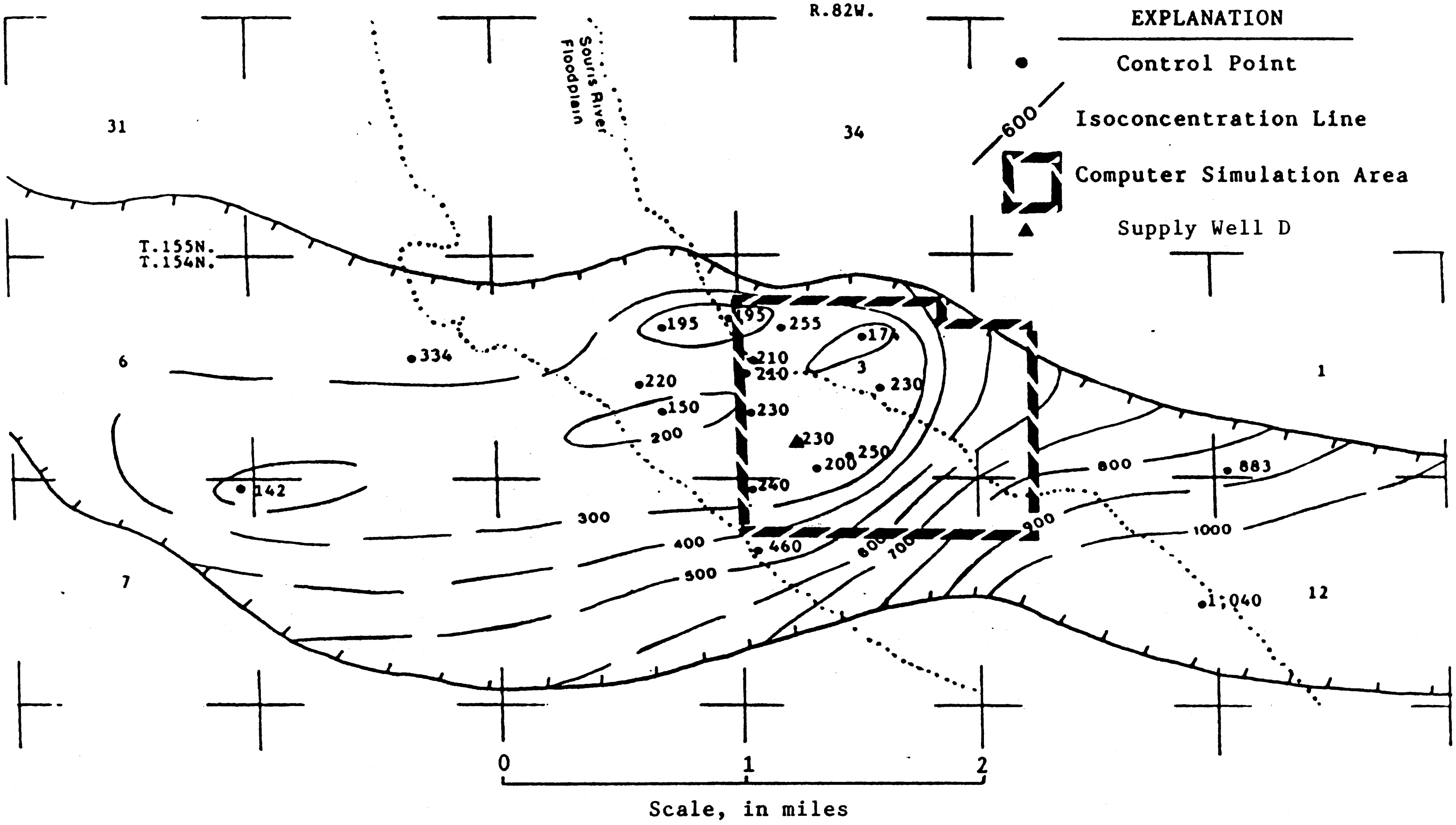


Figure 16. Sulfate Concentration Map, Pre-Development

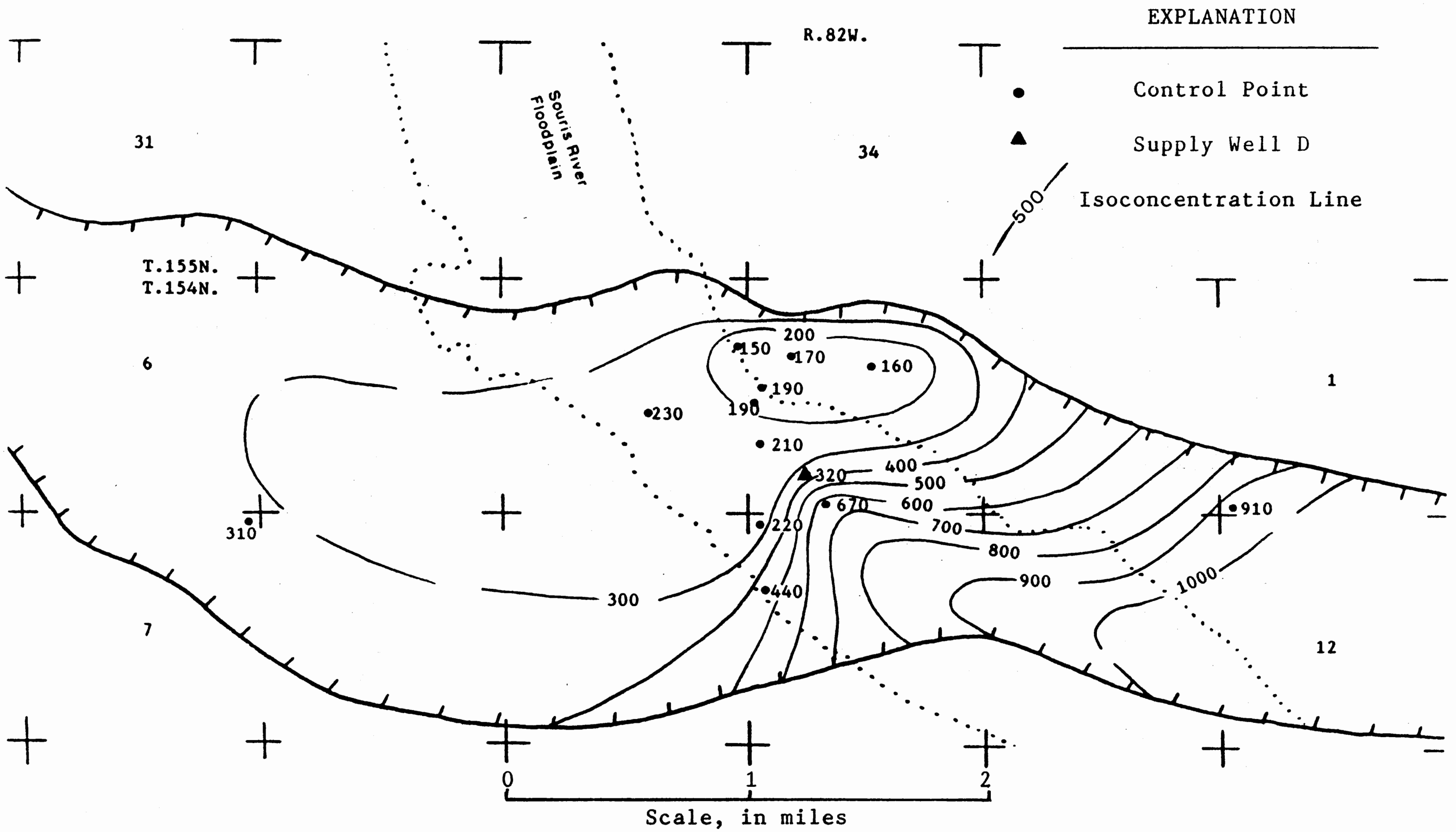


Figure 17. Sulfate Concentration Map for September, 1978

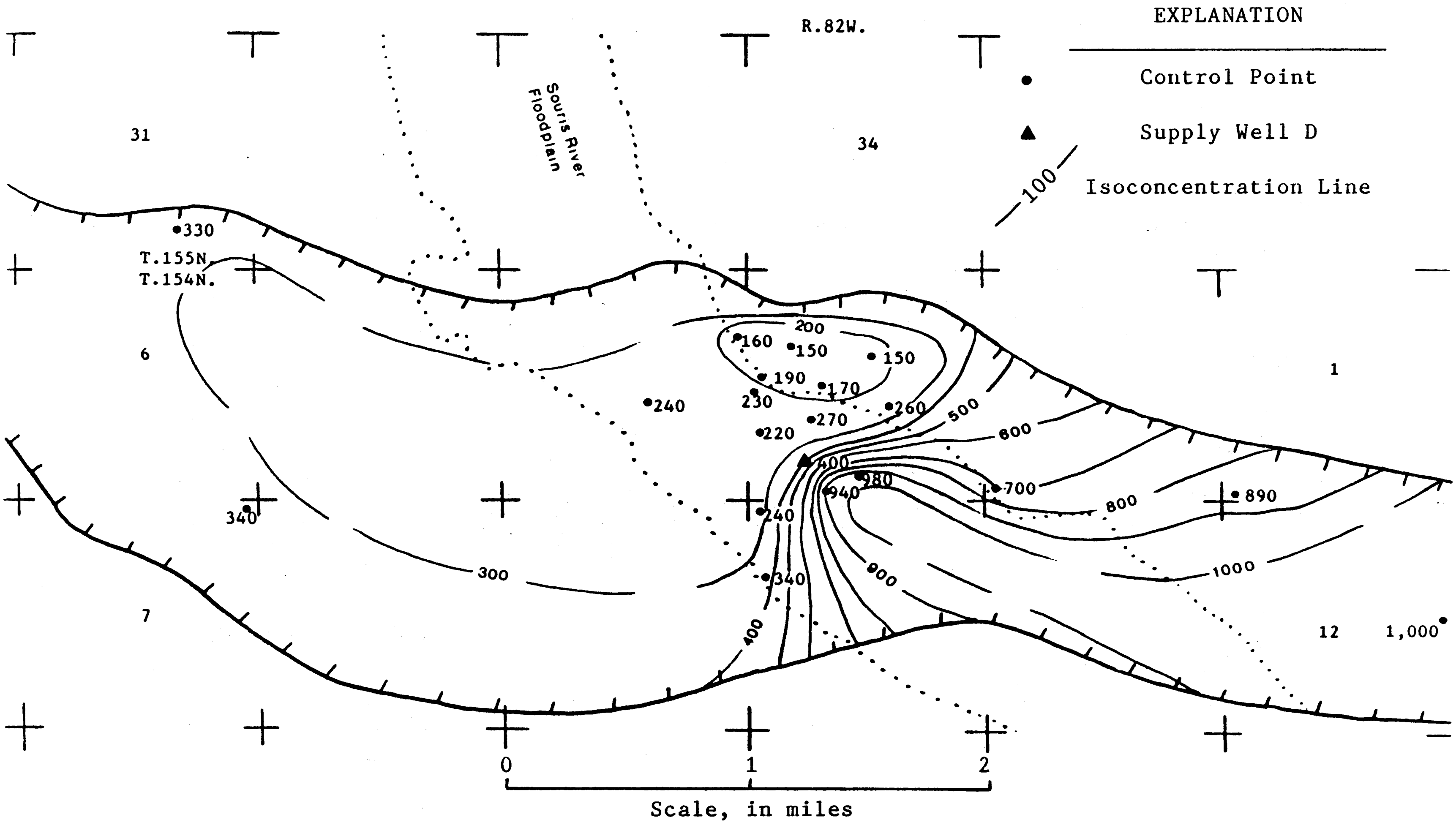
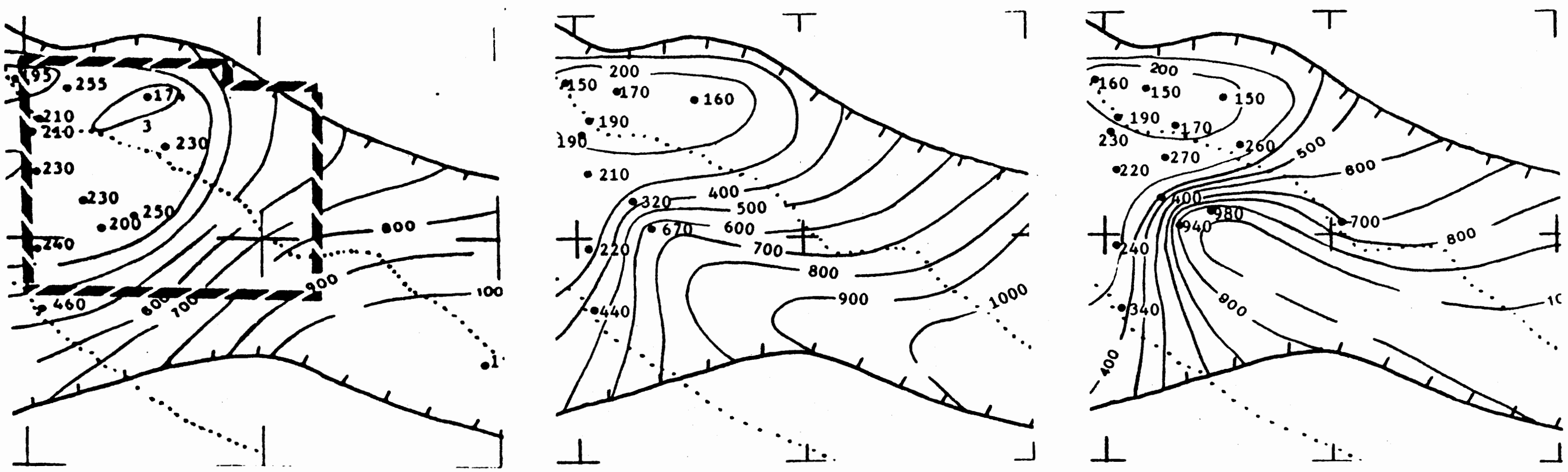


Figure 18. Sulfate Concentration Map for August, 1985



Pre-Development 1974

Post-Development 9-78

Post-Development 8-85

Figure 19. Contours of Sulfate Concentration Changing With Time

results in wells being located within 10 acre units, which correspond to a cell size of 660 by 660 feet.

As the model uses particles to represent the solute, a particle mass (PM) must be calculated for the given conditions according to the following equation.

$$PM = \frac{\text{Conc. * CDX * CDY * Thick * Poro. * 62.4}}{10^6 \text{ * No. Part.}} \qquad (2)$$

The end-member waters which mix within the Sundre aquifer are represented by the high sulfate water to the east of the well field and low sulfate water derived as recharge from the overlying Souris aquifer (figure 20). The leakage from the Souris aquifer is handled by the model through injection wells, located along the trend of the Souris aquifer. Two previous studies by Poore (1987) and Pusc (1987B), determined the leakage to be contributing up to 98% and 63%, respectively, of the water being removed due to pumping.

The model presents one particular problem, in its inability to represent no-flow boundaries. The Sundre aquifer is contained within the margins of a buried valley which is cut into the underlying bedrock. The high contrast between the transmissivity of the Sundre aquifer and the adjacent bedrock is best represented by a no-flow boundary. Without this boundary, the cone of depression from the well field does not extend along the trend of the aquifer as indicated by the potentiometric maps in Appendix B, which

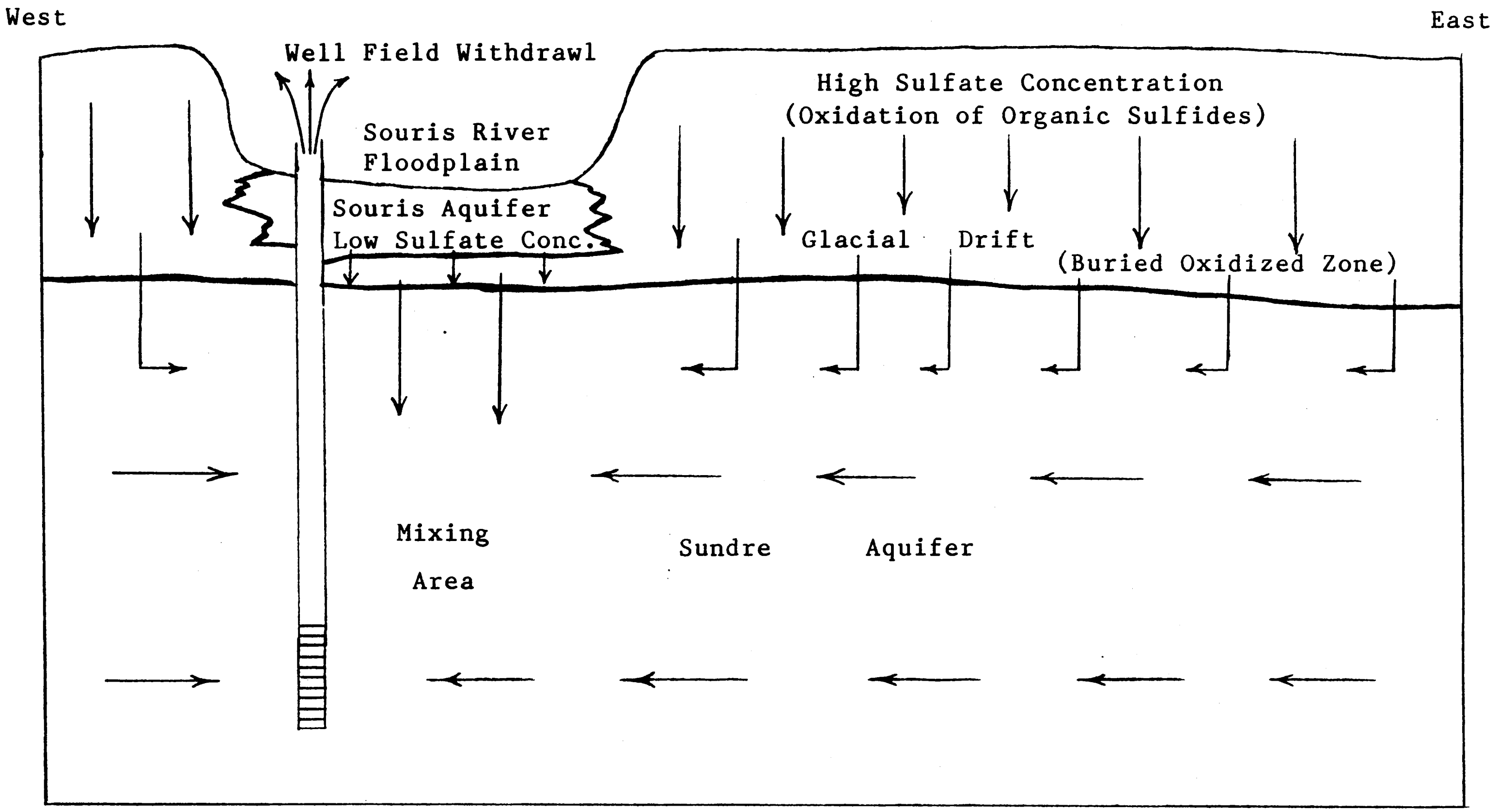


Figure 20. Conceptual Model of Sulfate Distribution

represent the aquifer after development of the well field. To help correct for this deficiency, particles representing sulfate are only placed within the confines of the Sundre aquifer.

The area which can be included in the simulation is controlled by the detail required. A larger area results in each particle having a larger mass to account for the increase in solute within the area, as the model is limited in the number of particles it can use. The original version of the model was limited to 1,000 particles. The model was modified to accept up to 2,000 particles, in order to reduce the particle mass assigned to each particle. The area simulated with the model is shown in figure 16.

The simulation began in 1976 and was advanced in time steps of one year, until 1986. The pump rates of each well were adjusted to the yearly average at the beginning of each time step. Pump rates for each well have been included in Appendix C. To maintain a constant source of sulfate, the eastern most column of particles was restored to a concentration of 1,000 mg/l at the beginning of each time step. Figure 16 indicates a background concentration of approximately 1,000 mg/l in the Sundre aquifer up-gradient from the well field.

Model Calibration

The calibration of the model was accomplished by adjusting the mass transport coefficients, and location and injection rates of the wells used to simulate recharge from the overlying Souris aquifer. A standard or goal should exist, against which some results of the simulation can be compared to evaluate the model performance. The standard used for calibration was the sulfate concentration at each production well over time. The concentrations computed for each well were compared against those found to exist at each well through periodic chemical analyses.

The early attempts with the model used the "average" values for the various hydraulic parameters discussed in Chapter V. With these values held constant, the injection wells were changed in number, location, and rate until the best calibration was obtained. This resulted in 5 injection wells with injection rates of 100,000 gallons per day at the locations shown in figure 21.

With the injection wells in place, the mass transport coefficients were varied to obtain the best calibration possible. DMAX, the distance which particles are moved before their velocity and vector are recalculated, was varied as a additional calibration tool. The capture radius of each production well was adjusted as a last step in the calibration process. The range of values attempted for each variable used in the calibration is provided in Table II.

The best calibration was produced with the mass transport coefficients and initial concentrations shown in figure 22. A DMAX value of 165 feet was used in the most accurate calibration. Well capture radiuses used for each well are

TABLE II

TABULATION OF CALIBRATION ATTEMPTS

Calibrated Variable	Range Attempted	Number of Attempts
Transmissivity (gpd/ft)	100,000 - 500,000	6
Hydraulic Conductivity (gpd/ft sq)	600 - 8,000	8
Storativity	.0001 - .06	5
Effective Porosity (percent)	10 - 40	5
Ground Water Velocity (X) (ft/day)	.1 - 1.2	6
Ground Water Velocity (Y) (ft/day)	0 - .2	3
Longitudinal Dispersivity (ft)	35 - 140	9
Transverse Dispersivity (ft)	7 - 28	3
DMAX (ft)	132 - 660	4
Well Capture Radius (ft)		
A	100 - 300	3
B	100 - 200	2
C	100 - 200	2
D	100 - 600	4
E	100 - 200	2

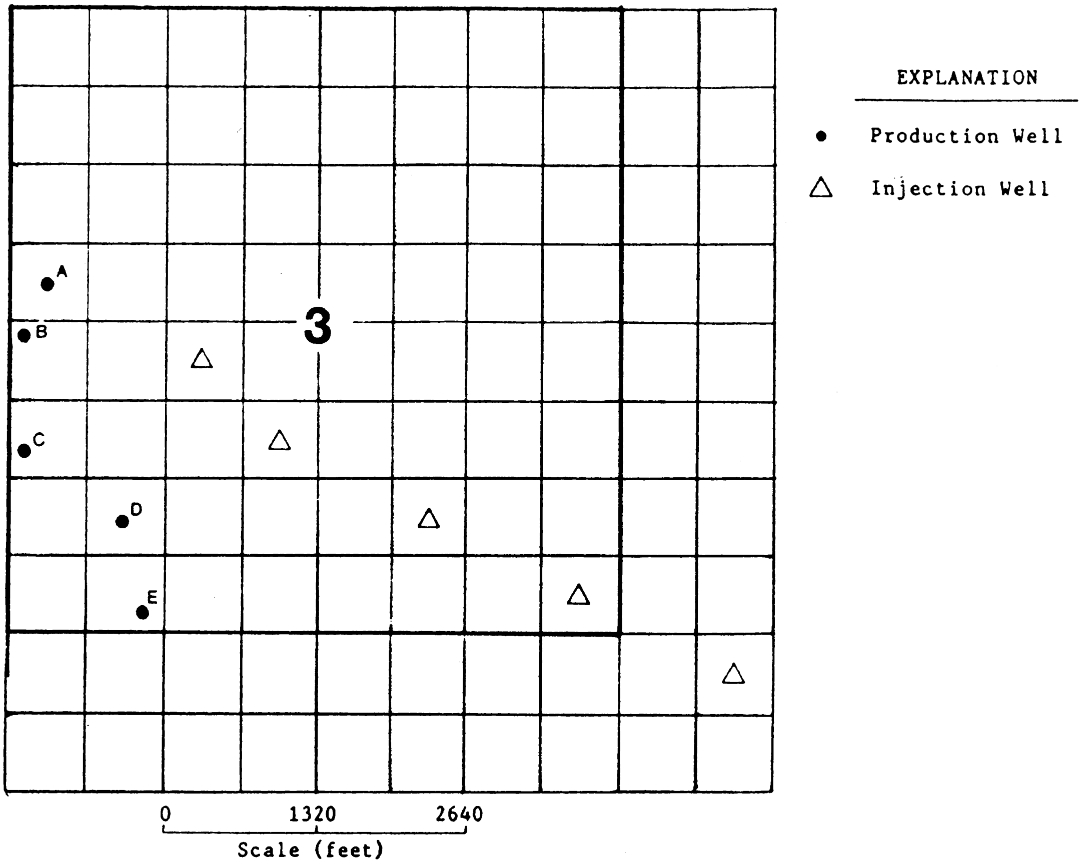


Figure 21. Computer Simulation Grid Map

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////////////PRESENT MASS TRANSPORT COEFFICIENTS\\\\\\\\\\\\\

             TRANSMISSIVITY =  200000  GPD/FT
             STORAGE COEFFICIENT   =  .0003
             HYDRAULIC CONDUCTIVITY =  2000  GPD/SQ.FT.
             POROSITY =  .25
             RETARDATION COEFFICIENT =  1
             REGIONAL X FLOW = -.5  FT/DAY
             REGIONAL Y FLOW =  .1  FT/DAY
             PARTICLE MASS =  16988.4  LBS
             DISPERSIVITY MODEL IS CONSTANT
             LONGITUDINAL DISPERSIVITY =  70  FT
             TRANSVERSE DISPERSIVITY =  14  FT

\\\\\\\\\\\\\\\\\\\\\\\\\\\///////////////////////////////

ACCUMULATED TIME =  0  DAYS      PARTICLES=  1666
CONCENTRATION MAP IN PPM (P SIGNIFIES PUMPAGE, I SIGNIFIES INJECTION)

    Y
66004   y   y   y   y   y   y   y   y   y   y   y
59404   y   y   y   y   y   y   y   y   y   y   y
52804   y   y   y   y   y   y   y   y   y   y   y
46204 200 300 350 400 600 700 700   y   y   y   y
39604 200 200 300 400 500 600 700 700 9001000   y     X AND Y COORDINATES
33004 200 200 200 300 300 400 700 700 9001000   y      SHOWN ARE IN FEET
26404 200 200 200 200 300 300 600 700 9001000   y         FROM ORIGIN
19804 200 200 200 200 200 300 500 700 9001000   y
13204 200 200 200 200 300 300 700 700 9001000   y
660 4 300 300 300 600 600 600 900 900 9001000   y
0   4 500 500 500 800 800 80010001000100010001000   y
     DDDBDDDBDDDBDDDBDDDBDDDBDDDBDDDBDDDBDDDBDDDB X

        0   6   1   1   2   3   3   4   5   5   6
            6   3   9   6   3   9   6   2   9   6
            0   2   8   4   0   6   2   8   4   0
                0   0   0   0   0   0   0   0   0
```

Figure 22. Mass Transport Coefficients and Pre-Development Sulfate Concentrations

as listed: well A 300 ft, well B 100 ft, well C 100 ft, well D 600 ft, and well E 200 ft.

The graphs showing the calibration results for each of the wells are shown in figures 23-27. The solid lines represent the actual sulfate concentration as it changes over time at each well. The dashed lines indicate the concentration as calculated by the model. The model was calibrated to provide the closest match for the D and E wells, as the D well is the most important due to its high production rate. On average, the D well supplies twice the production as the other wells combined.

The model calculated a sulfate level substantially lower for the A well than measured. The B well showed a erratic simulated level, over-estimating the sulfate level early and under-estimating it latter in the calibration period. The simulated concentration was consistently too low for the C well, with the difference averaging 70 mg/l. The model was able to predict the overall trend of the sulfate concentration for the D well, with the simulated level closely approximating the calculated level for most years. The E well had a erratic simulated level, which declined to 500-600 mg/l less than concentrations actually measured at the end of the calibration period.

Evaluation of the Model as a Predictive Tool

The calibration of the model serves a dual role. The first of which is to help adjust the variables the model

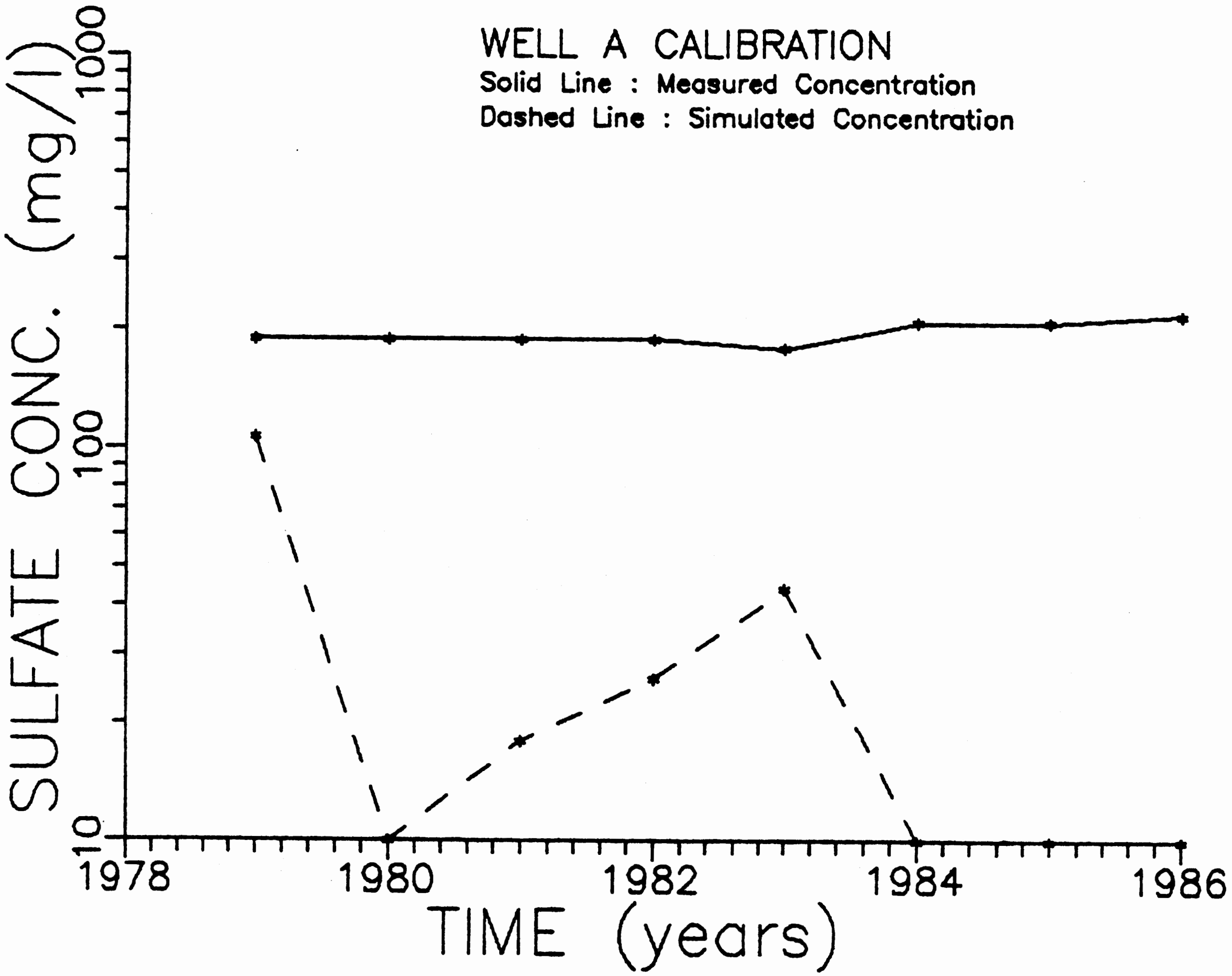

Figure 23. Calibration for Well A

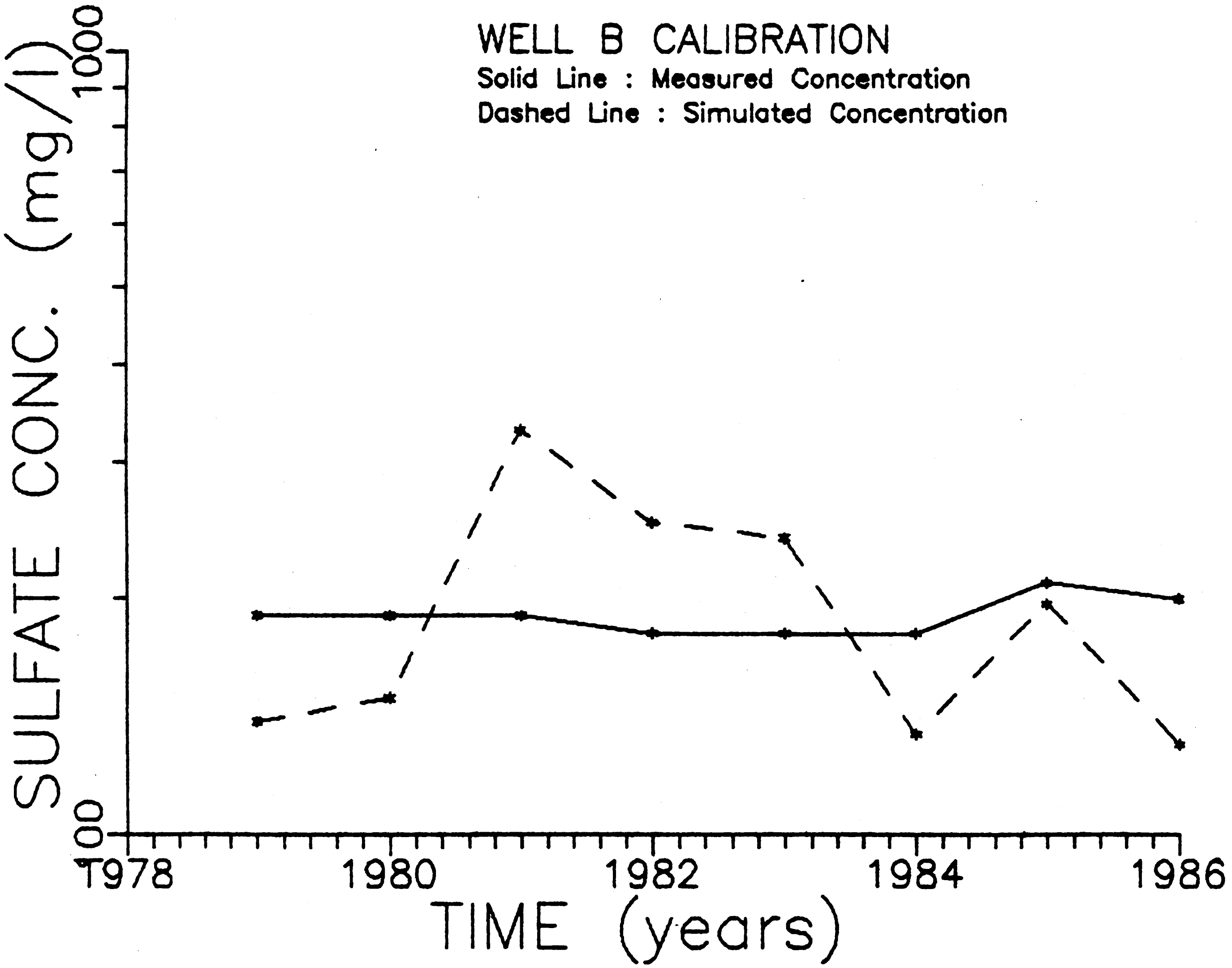

Figure 24. Calibration for well B

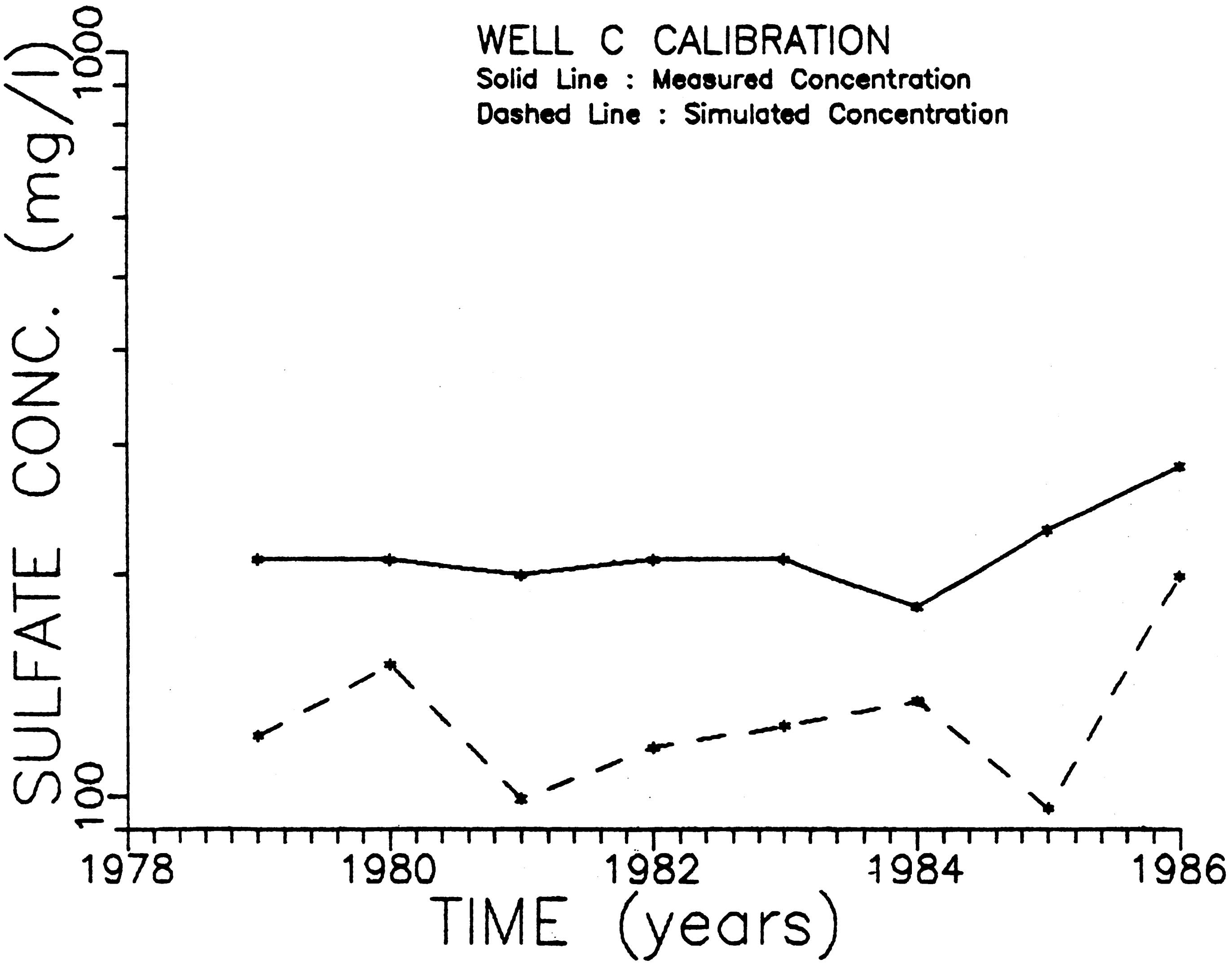

Figure 25. Calibration for Well C

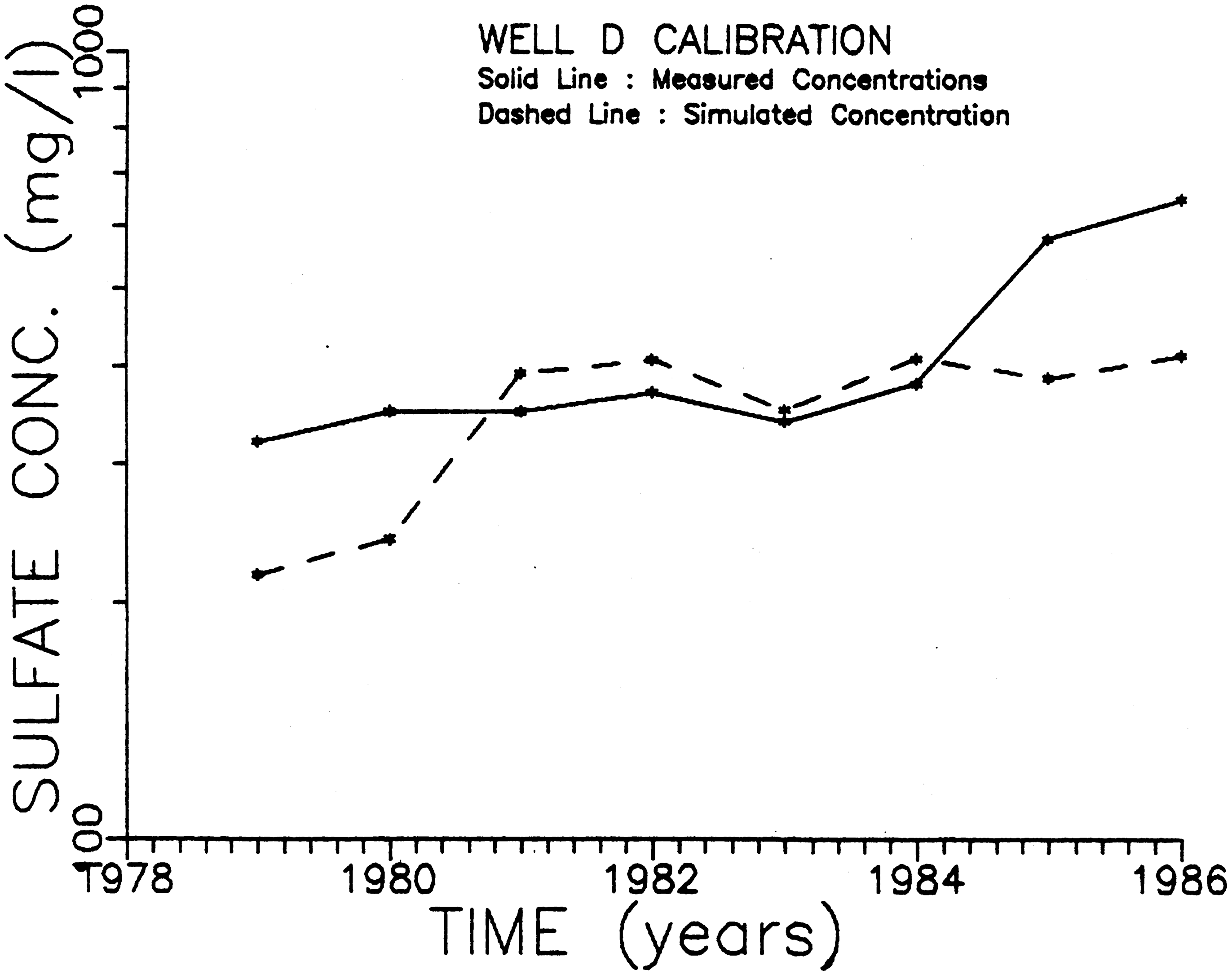

Figure 26. Calibration for Well D

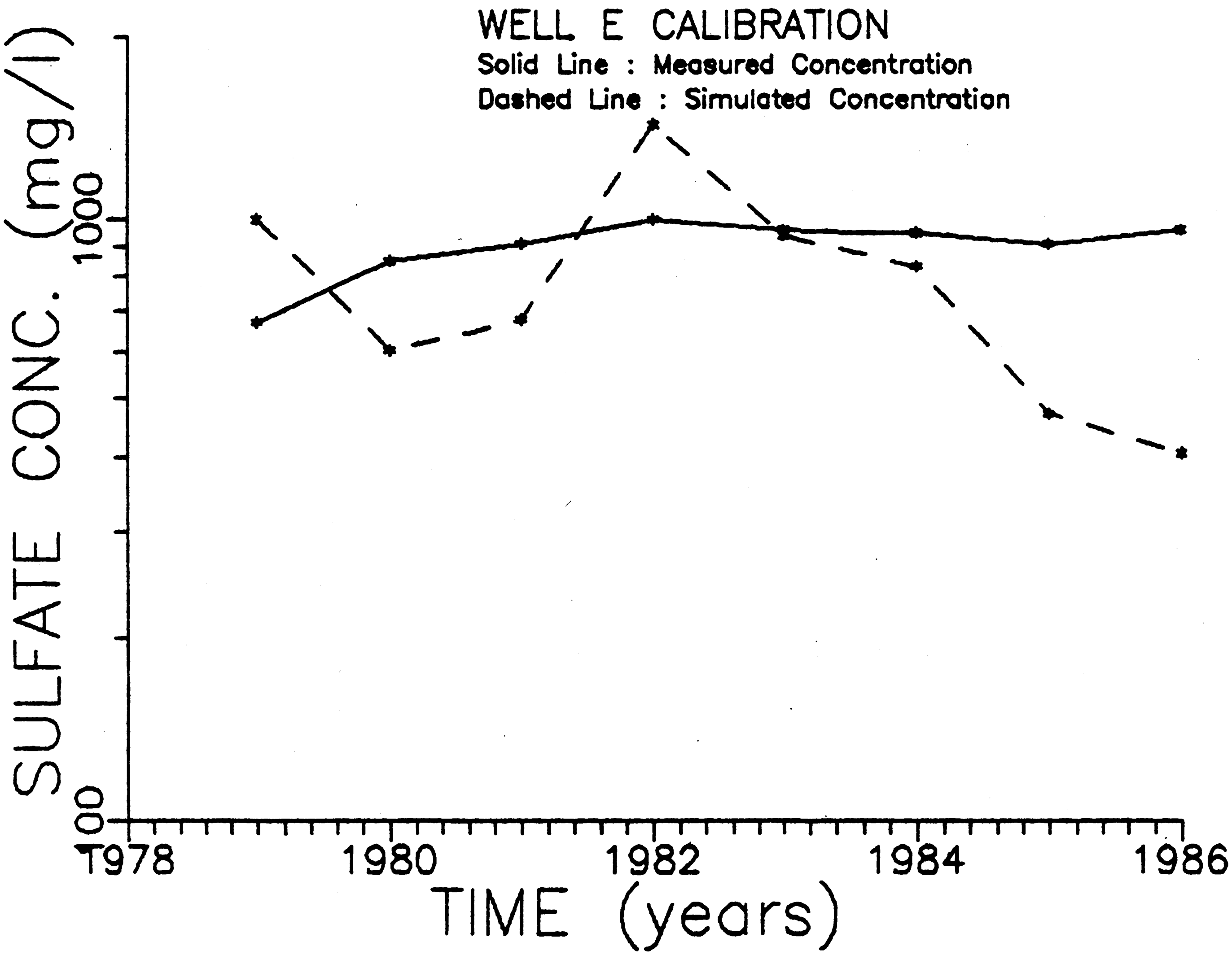

Figure 27. Calibration for Well E

utilizes in order to provide as close a simulation to reality as possible. The calibration also provides a indication of how well the model performed. The results indicate that the model might be useful for predicting only the concentration of the D well.

To further assess the model's predictive ability, it was used to simulate the sulfate levels for an additional simulation period (1987-1996). The production wells were pumped at an average rate, as determined from the calibration period (1976-1986). The model was advanced in yearly time steps, with particles added at each step to simulate a continuous source of 1,000 mg/l sulfate.

The concentrations as calculated by the model for wells B, C, D, and E are presented in figure 28. The model calculated a concentration of 0 mg/l for the A well. The trend for the D well appears possible, however, the model predicts the E well to have a concentration less than the D well. This is unreasonable, as the E well has maintained a substantially higher concentration than the D well since the inception of the well field. The B well shows a steady decline in concentration, which seems unlikely based on the steady concentration of the past.

The use of the model to predict future sulfate levels is not recommended. The inability of the model to perform satisfactorily is most likely the result of the model assuming homogeneous and isotropic conditions. The Sundre aquifer contains large heterogeneities which the model is

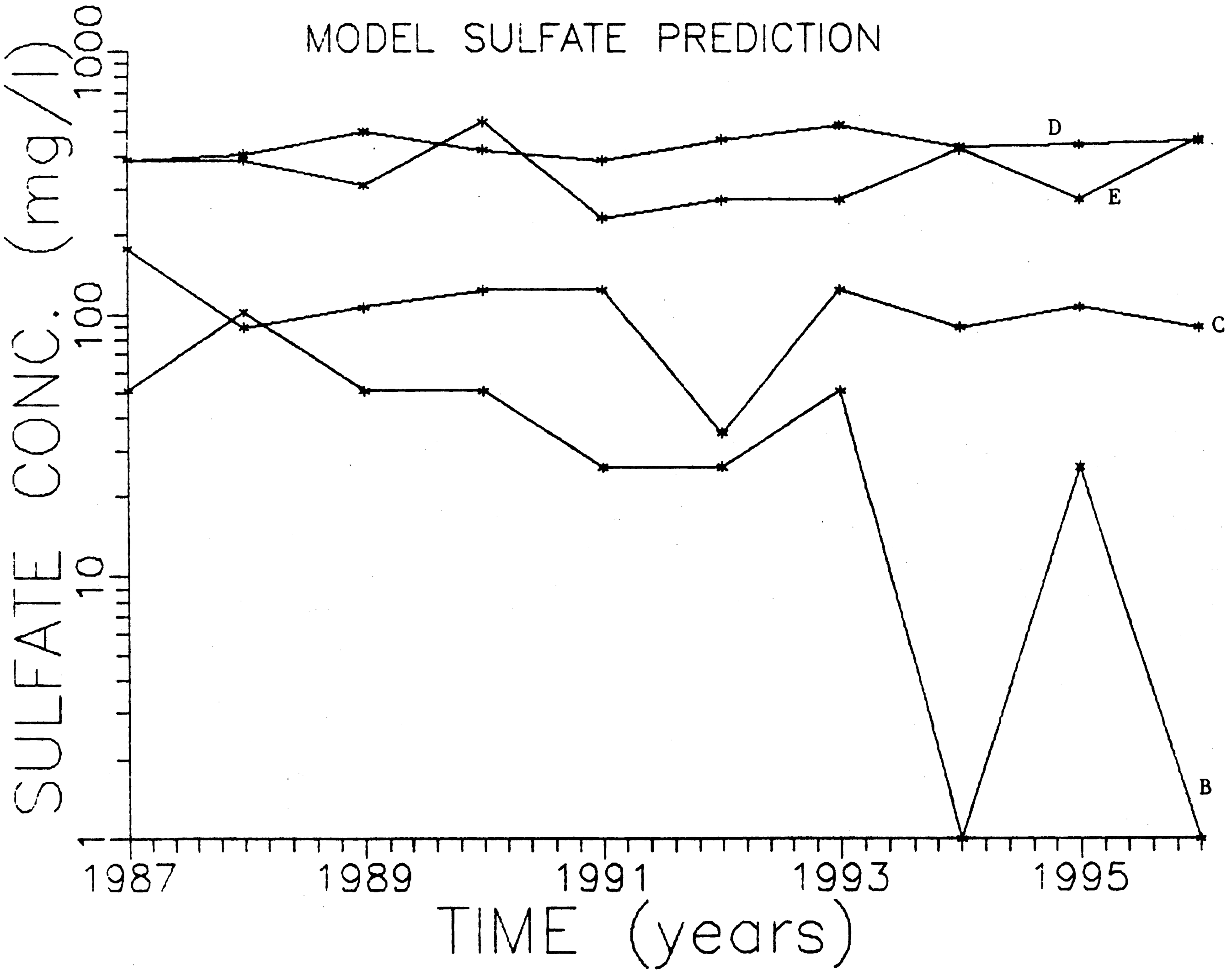

Figure 28. Model Sulfate Prediction for 1987-1996

unable to simulate.

Sensitivity Analysis

The computer model was tested for its sensitivity to changes in assigned mass transport coefficients (figure 22). The following discussion details the effects of varying the mass transport coefficients, up or down, from the assigned values.

A increase in the hydraulic conductivity produced irregular results. The concentration decreased in the B, D, and E wells. A increase in concentration occurred in wells A and C. These results are considered irregular, due to the fact that wells A and B, which are located close to each other had opposite reactions to the increase in hydraulic conductivity. A decrease in hydraulic conductivity produced a reversed change in concentration in each well.

The transmissivity (T) is related to the hydraulic conductivity (K) by the aquifer thickness (b); $T = K * b$. Changing the transmissivity, while holding the hydraulic conductivity constant, effectively varies the aquifer thickness. Increasing the transmissivity resulted in decreased concentrations throughout most of the well field. A increase in concentration occurred when the transmissivity was decreased.

Variations in the storativity appeared to have little or no affect on the sulfate concentration. Increasing the storativity lessens the change in the potentiometric head for the withdrawal of a given volume of water. A decrease in storativity has the opposite effect.

Increasing the ground-water velocity up to the expected maximum of 1.2 ft/day increased the concentration toward the southern end of the well field. The increase was most notable in wells D and E. Wells A and B, located to the north, showed a decrease in concentration. No change in concentration occurred in the northern end of the well field when the velocity was decreased. The southern end of the well field experienced a decline in concentration when the velocity was reduced.

The longitudinal and transverse dispersivities appeared to effect similar changes in sulfate concentration. The sulfate concentration increased toward the southern end of the well field, when either the longitudinal or transverse dispersivities were decreased. This change resulted in a slight decrease in concentration toward the northern end of the well field. A increase in the longitudinal dispersivity produced a slight decrease in concentration toward the southern wells, while little change occurred in the northern wells. The sulfate concentration decreased in the southern end of the well field when the transverse dispersivity was increased. Increasing the transverse dispersivity produced a slight increase in concentration in the northern end of the well field.

The results of the sensitivity analysis indicate that the model is most sensitive to adjustments in the hydraulic conductivity. This suggest potential problems with the simulation, as the hydraulic conductivity for the entire study area is based on one pumping test.

CHAPTER VII

CONCEPTUAL MODEL - COMPUTER MODEL INTERFACE

Introduction

The success of the interface between the conceptual model and computer model determines the utility of the computer model. Computer models commonly have limitations which impair the interface between the two models. If a inaccuracy exist in the conceptual model, this will reduce the accuracy of the computer model. These problems are discussed below as they pertain to the Sundre aquifer simulation. The inability of the computer model to perform satisfactorily is suggested to be the result of these problems.

Sulfate Distribution

The sulfate levels in the eastern extension of the Sundre aquifer increase evenly in a easterly direction (figure 16). The sulfate level rises to approximately 1,000 mg/l near the eastern margin of the study area. This distribution was entered into the computer model as shown in figure 22. The sulfate concentration may not be as evenly distributed as indicated, due to heterogeneities in the vertical hydraulic conductivity. Areas with increased vertical hydraulic conductivity may have elevated sulfate levels due to greater recharge from the overlying oxidized till horizon. Abnormal sulfate distributions should not pose a significant problem, however, due to dispersion within the aquifer. Mixing, as the result of dispersion, will dilute locally elevated sulfate concentrations.

As discussed in Chapter IV, recharge from the overlying Souris aquifer dilutes the sulfate concentration in the vicinity of the well field. Prior to development of the well field, the regional hydraulic gradient was to the west. This resulted in reduced sulfate levels in the western extension of the Sundre aquifer (figure 16). The development of the well field reversed the hydraulic gradient, such that water now flows from the western extension of the Sundre aquifer towards the well field. The sulfate level in the western extension of the aquifer should rise, as recharge from the overlying oxidized till horizon is no longer being diluted by fresher waters from the Souris aquifer. Examination of well 154-082-7AAA before and after development of the well field confirmed the rise in sulfate concentration. The sulfate level increased from 142 mg/l prior to development, to 340 mg/l eight years after development of the well field.

The computer model was evaluated using a constant source of sulfate to the east and west of the well field.

The model calculated higher sulfate levels for the northern wells, however, they were still under observed levels. No improvement was noted in the E well, in which the model errantly calculated a drop in the sulfate level towards the end of the simulation period. The concentration in the D well appeared erratic. The best calibration was obtained using only the eastern source, as presented in Chapter VI.

Presently, the sulfate levels immediately west of the well field are low relative to those east of the well field. This can be expected to change, making the addition of a western source of sulfate a viable option at some latter date.

The injection wells used to simulate recharge from the overlying Souris aquifer are injecting water with a sulfate concentration of 0 mg/l. The concentration in the Souris aquifer averages 100 mg/l. The model is not capable of assigning a concentration to the injection wells. This is accomplished by adding particles periodically to the cell in which the well is located. With a particle mass of 16,988.4 lbs., it is not practical to attempt adding particles. The addition of one particle created a greater concentration than required. The injection rates of the wells were adjusted to account for the injection of water with a sulfate concentration of 0 mg/l. This resulted in a lower injection rate, than if the injected water had a sulfate concentration of 100 mg/l.

Sulfate Transport

The potential for a significant problem in the interface between the two models exist when using an analytical model. The large variation in clast size in the Sundre aquifer suggests the potential for a large variation in the hydraulic conductivity. These heterogeneities are not accounted for by the computer model. Areas of higher hydraulic conductivity may provide preferred paths of migration for the high sulfate levels east of the well field. Wells located in or near areas of high hydraulic conductivity may experience higher sulfate levels than simulated by the model.

The decline in the sulfate concentration in well E towards the end of the calibration period (figure 27) may be attributed to a interface problem between the conceptual and computer models. The computer model is unable to simulate no-flow boundaries, such as exist along the southern boundary of the Sundre aquifer (figure 16). The model assumes the aquifer to be of infinite areal extent. The no-flow boundary forces the cone of depression from the well field to extend along the trend of the aquifer (Appendix B). This facilitates the transport of high sulfate waters, located to the east, toward the supply wells. The computer model, without a no-flow boundary allows water to be drawn from south of the aquifer boundary, where low sulfate waters occur. This produces a drop in simulated sulfate levels once these low sulfate waters reach the well. The E well, located the furthest south is affected the most. A similar situation exist along the northern boundary of the Sundre aquifer, and offers a possible explanation for the low simulated sulfate levels in well A. Well A is the furthest north well (figure 5). The problem is worse in well A than in well E, as would be expected since well A is located closer to the no-flow boundary. Well B appears to be subject to this same problem, as shown by its declining sulfate concentration (figure 28).

The use of image wells was evaluated as a means to incorporate no-flow boundaries into the analytical model. To represent no-flow boundaries, wells are placed an equivalent distance from the no-flow boundary but on opposite sides and are shown to be discharging at equal rates. It would be necessary to add image wells, for both the north and south no-flow boundaries, for each production well. This would require increasing the size of the computer simulation area to nearly four times its current size. As a result of this increase in areal coverage, the particle mass would increase to approximately 60,000 lbs/particle. The calibration of the model becomes difficult with such a large particle mass, due to the model calculating erratic concentrations.

The decision to use the model with the smaller computer simulation area and no image wells benefits the D well, at the expense of the A and E wells. The fact that the D well

supplies twice the production of the other wells combined dictates its importance.

CHAPTER VIII

SUMMARY AND CONCLUSIONS

Summary

The chemical analyses of water samples collected from the Sundre well field are characterized by unusually high sulfate levels. The sulfate was determined to be the result of the oxidation of organic sulfides, which occur in lignite. The lignite is widely dispersed throughout the surficial and bedrock geologic materials.

The Sundre well field had initial sulfate concentrations of 250 mg/l or less. Within 3 years, the sulfate level had risen to 670 mg/l in well E, the southernmost well. Located to the north of well E, well D showed an increase in the sulfate concentration to 320 mg/l. Wells A, B and C, located farther to the north did not show an increase in sulfate. This evidence suggested mixing of waters taking place within the Sundre aquifer.

A investigation into the possibility of mixing was conducted with the aid of Piper plots and the computer program BALANCE. Both of these tools confirmed the probability that mixing of waters was taking place within the Sundre aquifer in the vicinity of the Sundre well field.

Further evidence was discovered when studying the effect of the pump rate of the D well on the sulfate concentrations in the D and E wells.

The mixing is taking place between two end-member waters, represented by low sulfate water derived by leakage from the overlying Souris aquifer and high sulfate water in the Sundre aquifer to the east of the well field. The high sulfate waters east of the well field are the result of oxidation of organic sulfides present in till which overlies the Sundre aquifer. The natural mixing is augmented by the high withdrawal rate of the D well, which acts to draw water from both end-member sources. This results in the D well providing a representative mix of the two end-member waters.

The solute-transport model "Random-Walk" was evaluated as to its ability to simulate movement of sulfate within the Sundre aquifer. The model was calibrated through adjusting the aquifer coefficients, and the location and injection rates of wells used to simulate the recharge from the overlying Souris aquifer. The sulfate concentrations measured at the five production wells over time were compared against the concentrations calculated by the model during the same time period to assist in the calibration. The simulation period was for 1976-1986.

The degree to which the model was able to produce concentrations similar to those measured in the field indicated its performance. The model was only able to simulate the trend for the D well, with erratic concentrations calculated for the other wells.

To assess the model's predictive abilities, it was used to simulate the sulfate level for an additional simulation period (1987-1996). Average pump rates for the calibration period (1976-1986) were used for the simulation. The model indicated the E well to have a concentration lower than the D well. This appears unlikely, as the E well has maintained a substantially higher concentration since the commencement of pumping in the well field. The model's use as a predictive tool is not recommended.

The poor performance is thought to be due in part to the model's being limited to homogeneous and isotropic conditions. The Sundre aquifer is characterized by large heterogeneities, which could best be handled by a numerical model. The heterogeneities are simulated in numerical models through adjusting the hydraulic parameters in each cell to approximate actual conditions in the aquifer. To utilize the capabilities of a numerical model more hydraulic data are required than is currently available. This information could be obtained through slug tests or pumping tests carried out at each available well or test hole.

A sensitivity analysis conducted on the model indicated that it is most sensitive to changes in the hydraulic conductivity. The fact that the hydraulic conductivity is based on one pumping test suggests the potential for problems.

The potentially most significant problem encountered with the computer model was its assumption that the aquifer is of infinite areal extent. In fact, the aquifer is bounded by no-flow boundaries on the north and south. The omission of these no-flow boundaries by the model allows low sulfate waters to be drawn from the north and south. This results in the model's calculating sulfate levels that are too low in the wells located furthest north and south. A solution to this problem was evaluated with the incorporation of image wells to represent the no-flow boundaries. In order to add the image wells, the computer simulation area had to be increased to nearly four times its current size. The increase in study area, which required an increase in the particle mass to nearly 60,000 lbs/particle, resulted in great difficulty in calibrating the model. The decision was made to retain the smaller study area, which provided the most accurate calibration for the D well. The D well is considered to be the most important, due to its production being twice that of the other wells combined.

Conclusions

The following conclusions have been reached as a result of this study:

1. The source of sulfate in the Sundre aquifer was the oxidation of organic sulfides in the till horizon.

2. Mixing of waters is taking place within the Sundre aquifer, in the vicinity of the Sundre well field. The end-member waters consist of high sulfate waters to the east and

west of the well field, and low sulfate waters derived by recharge from the Souris aquifer, which overlies the well field.

3. There are difficulties involved in using the analytical version of the solute-transport model "Random-Walk" to model the movement of sulfate in the Sundre aquifer. The Sundre aquifer is inclined to have large variations in the hydraulic conductivity, which the model cannot account for. The Sundre aquifer is bound by no-flow boundaries on the north and south, which the model cannot simulate without the addition of image wells. The complexities of the Sundre aquifer could best be modeled with a numerical model.

4. Additional hydraulic data would be required to fully utilize the capabilities of a numerical model. This data could be obtained by performing pumping tests or slug tests on all available production wells or test holes.

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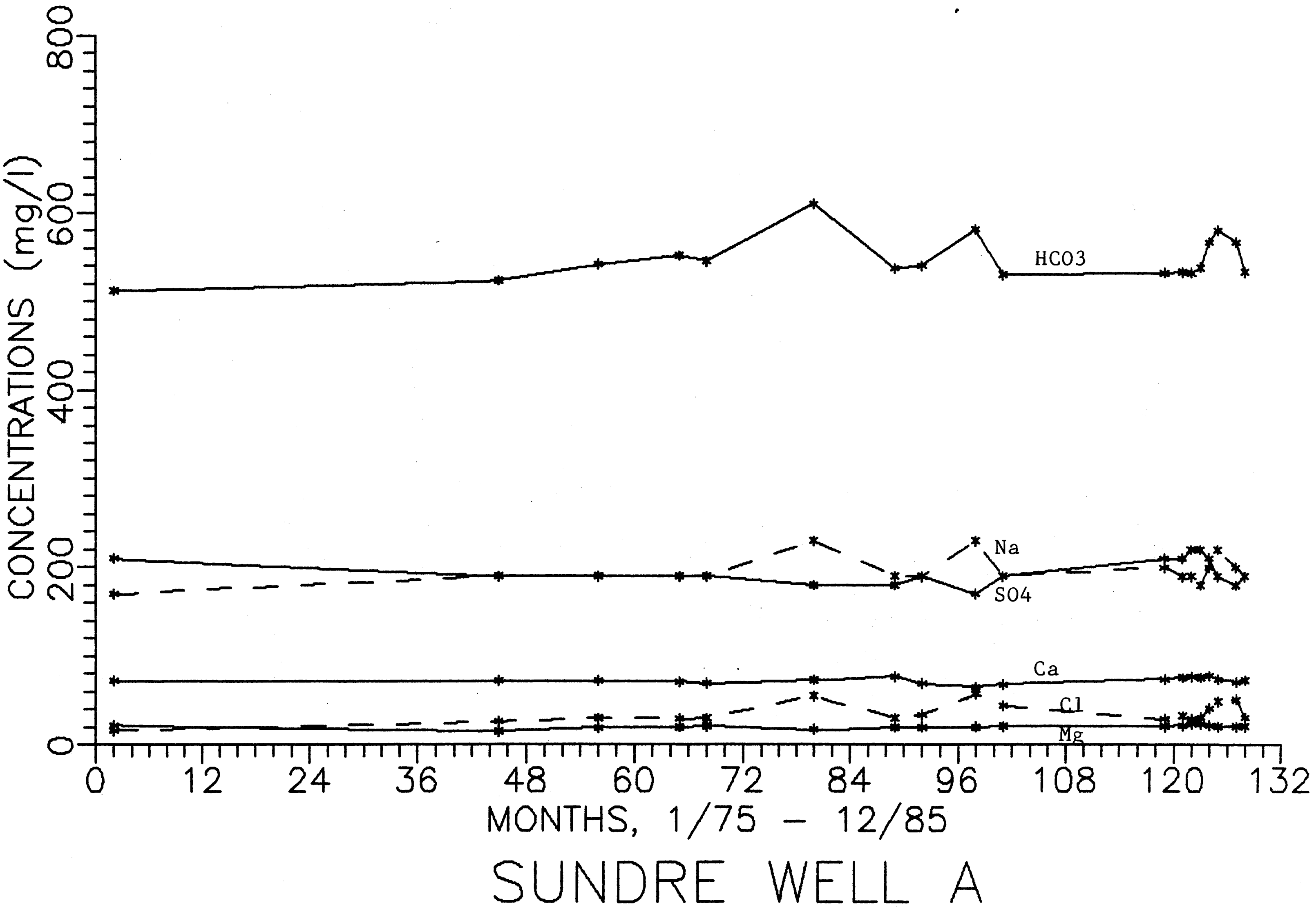
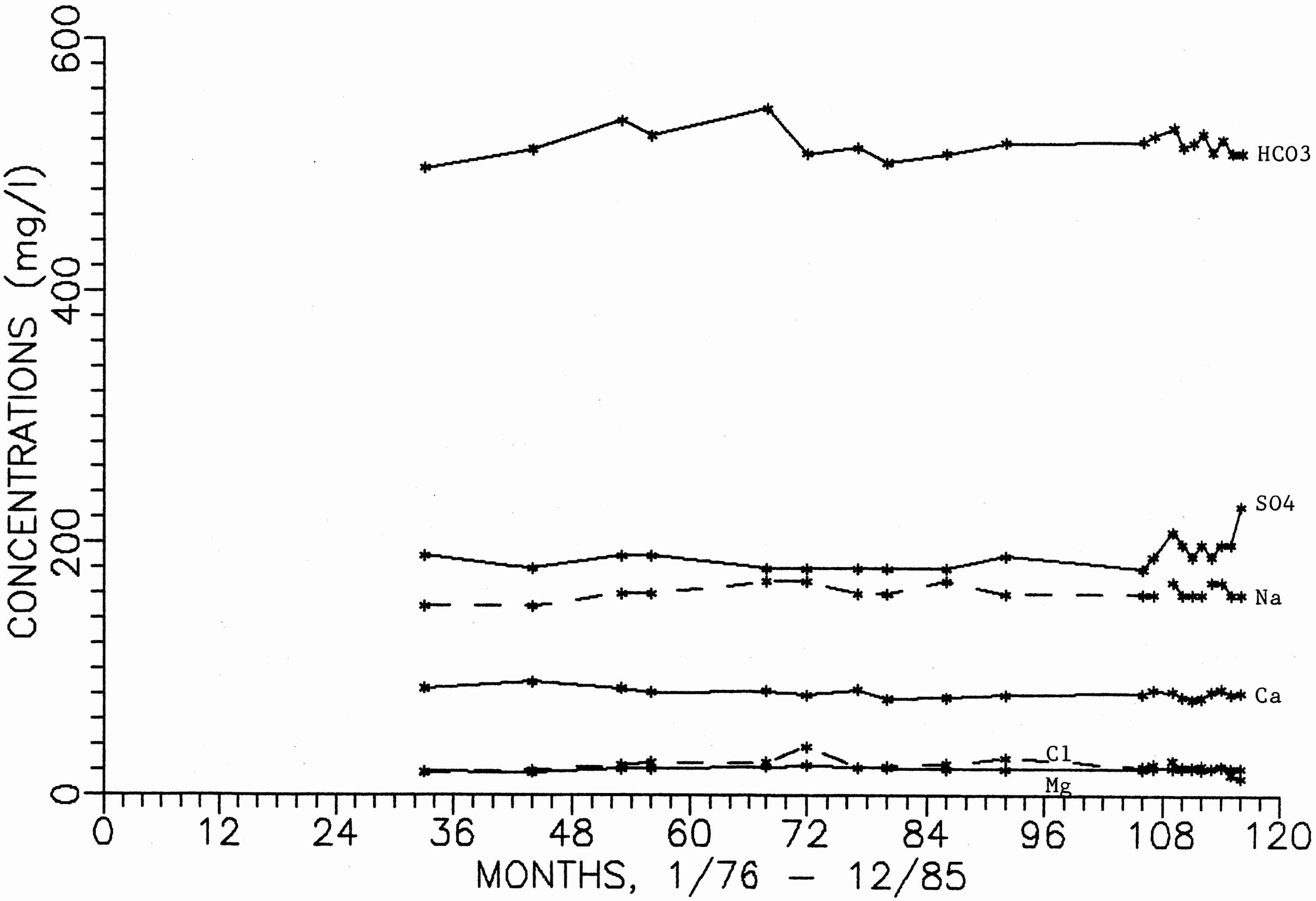
APPENDIXES

APPENDIX A

ION CONCENTRATIONS FOR PRODUCTION WELLS A-E


800
600
400
200
0
CONCENTRATIONS (mg/l)
0
12
24
36
48
60
72
84
96
108
120
132
MONTHS, 1/75 – 12/85
HCO3
Na
SO4
Ca
Cl
Mg
SUNDRE WELL A



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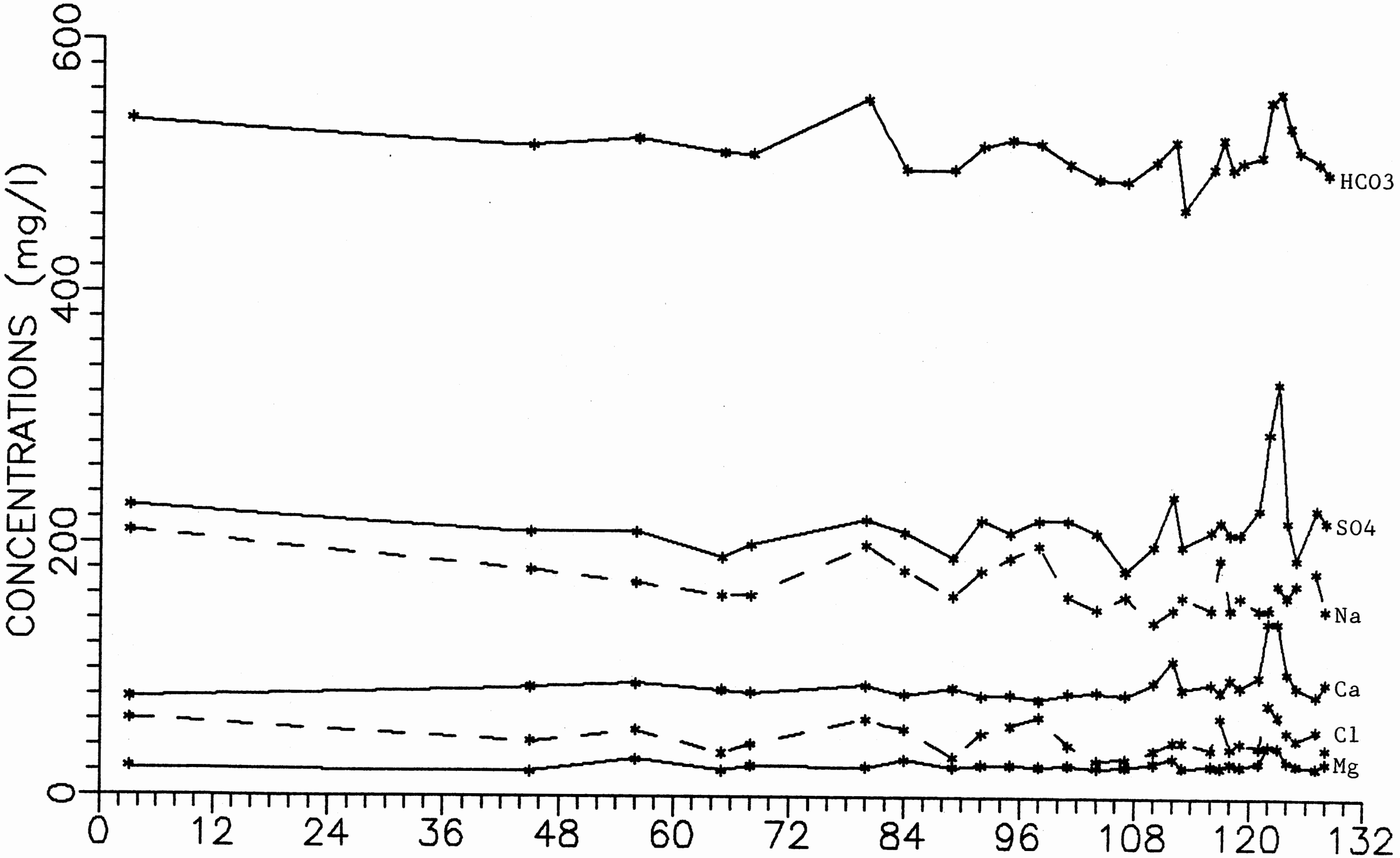

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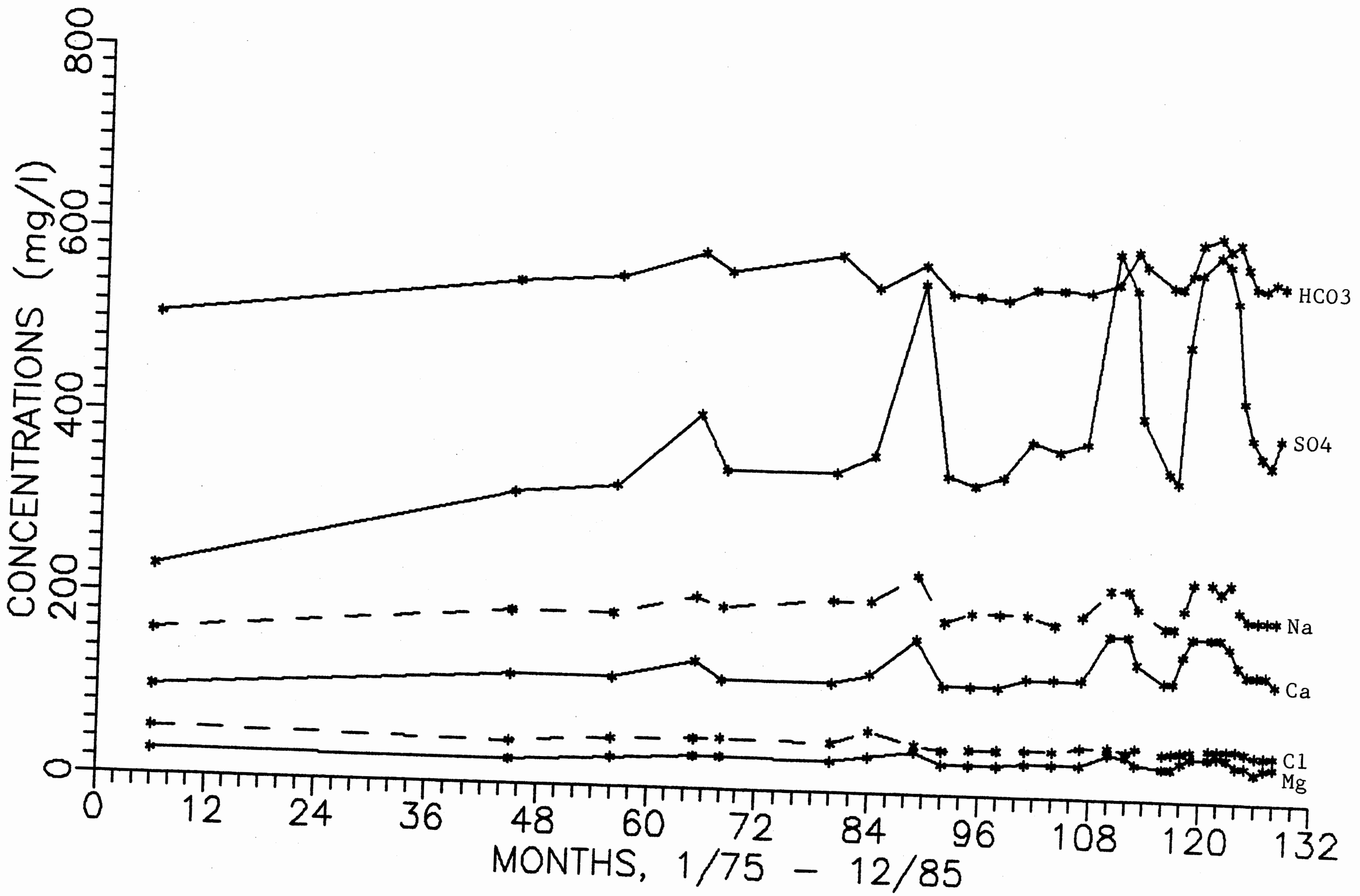

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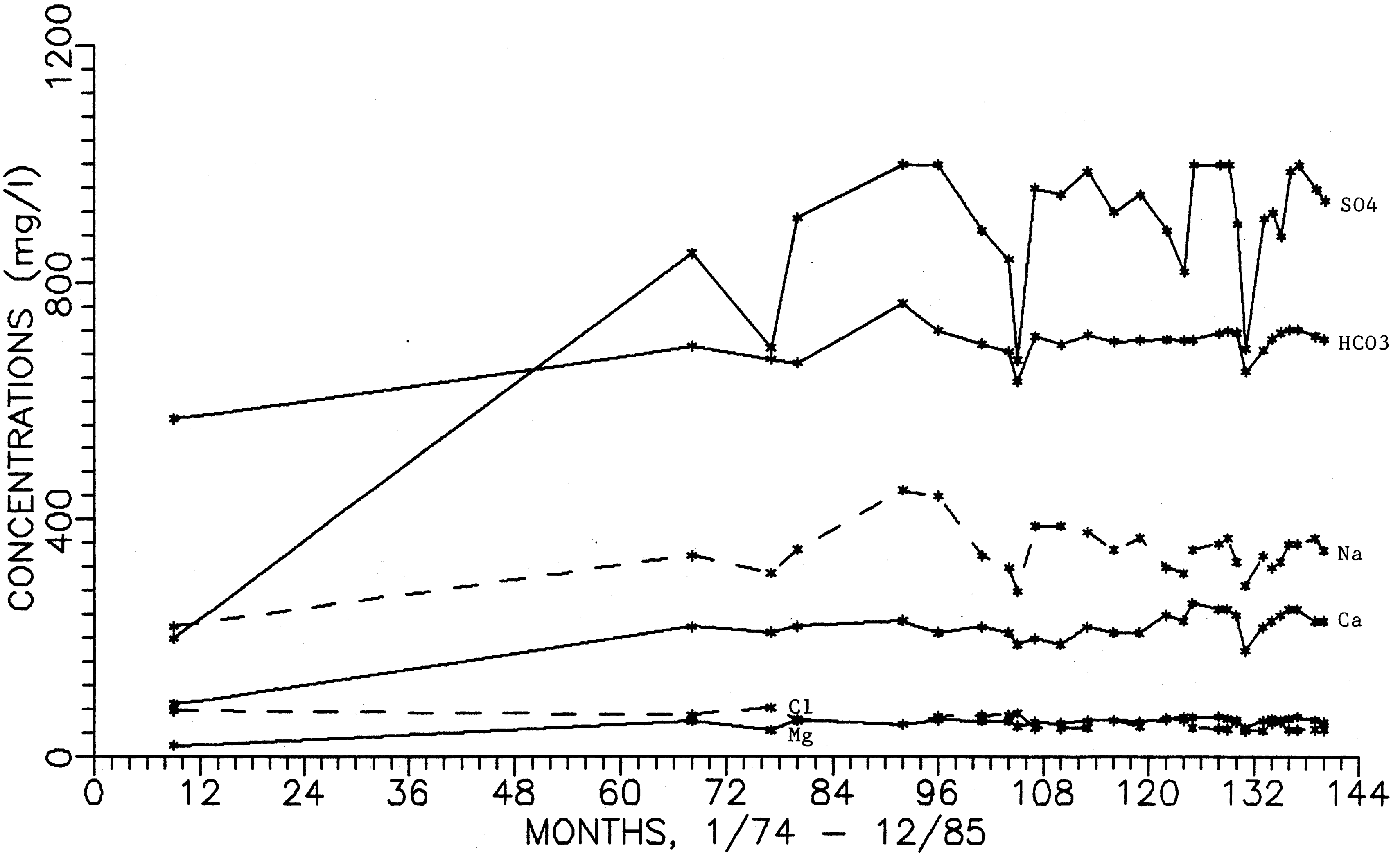
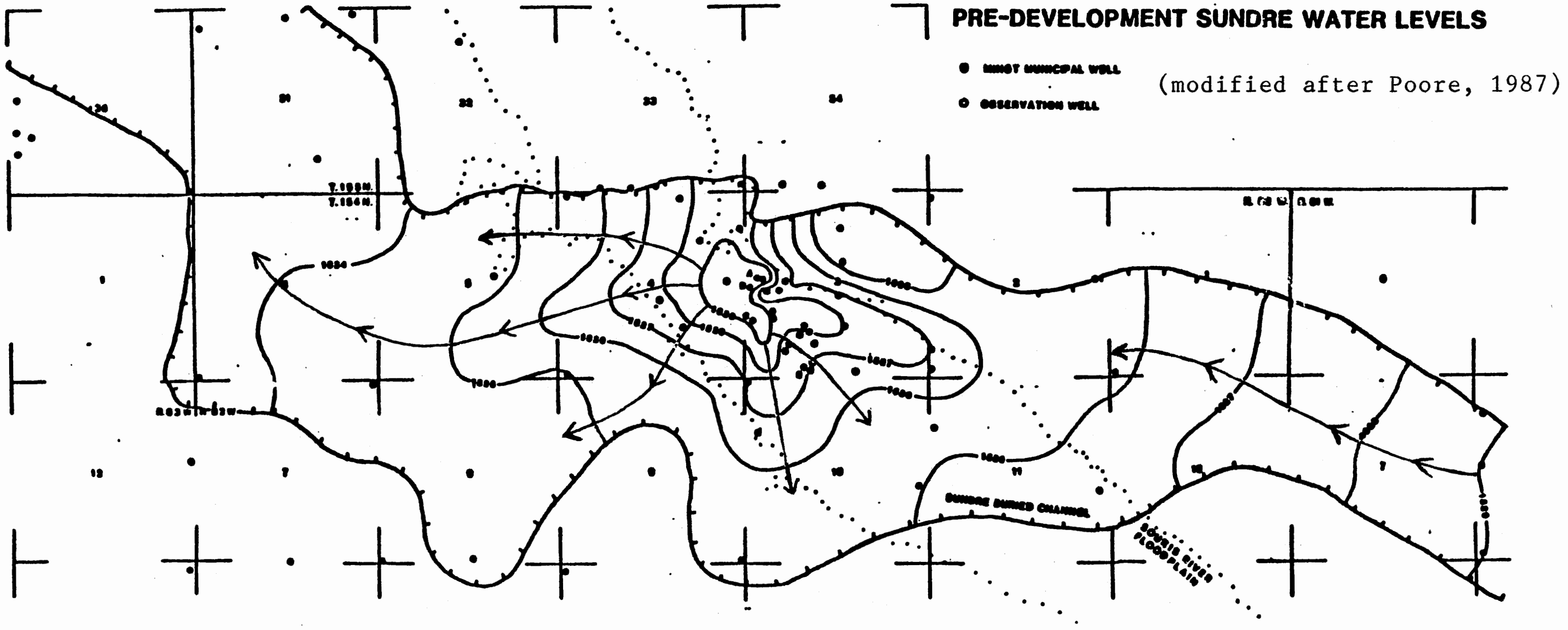


SUNDRE WELL E

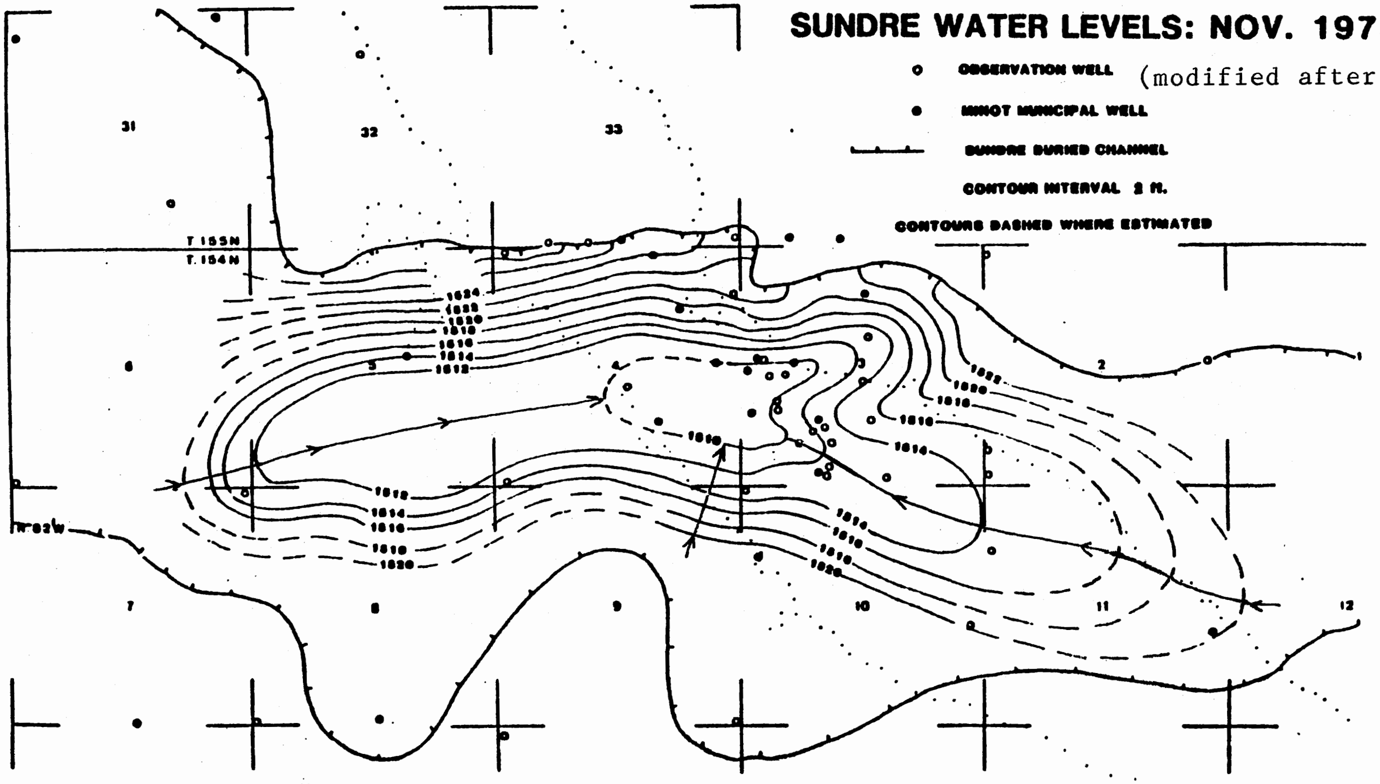
APPENDIX B

PIEZOMETRIC MAPS FOR SUNDRE AQUIFER



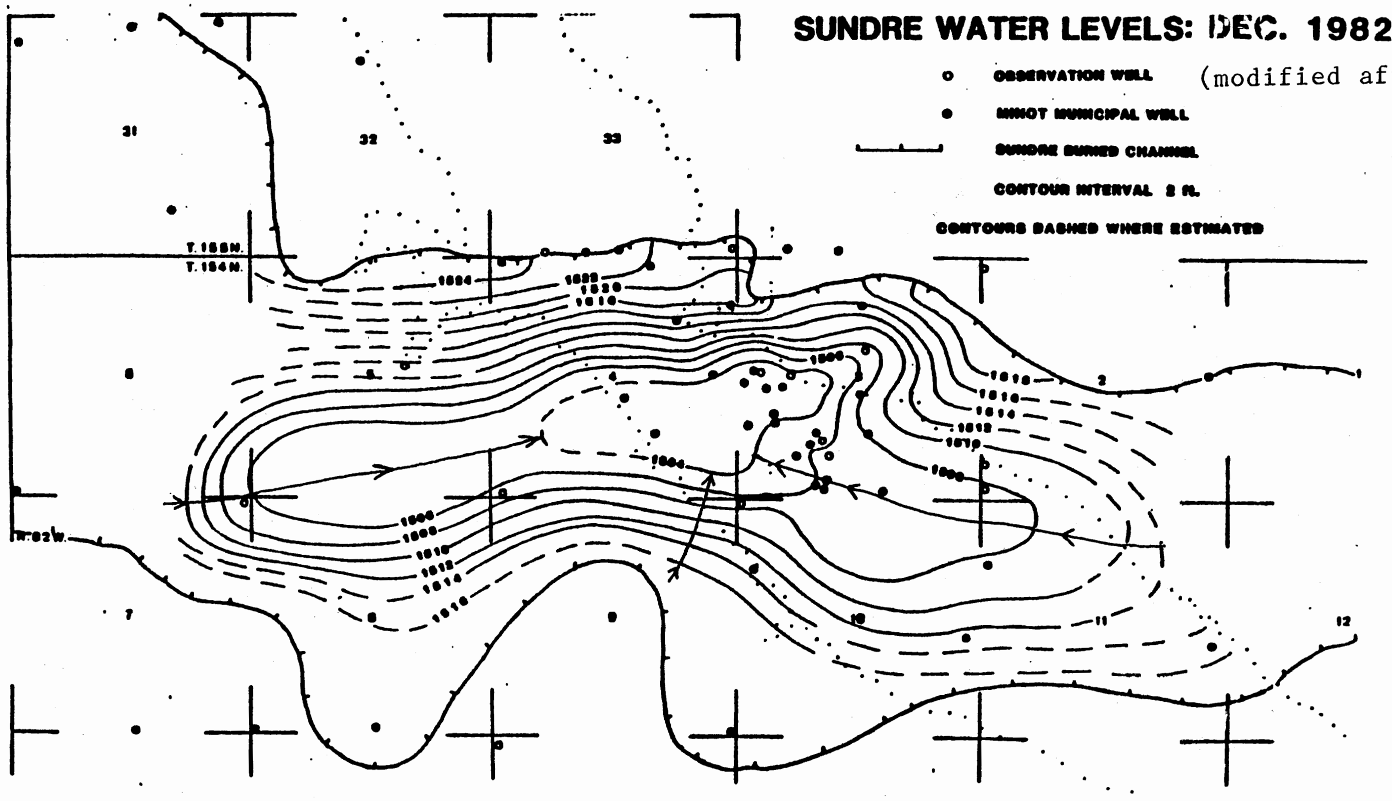
PRE-DEVELOPMENT SUNDRE WATER LEVELS

(modified after Poore, 1987)



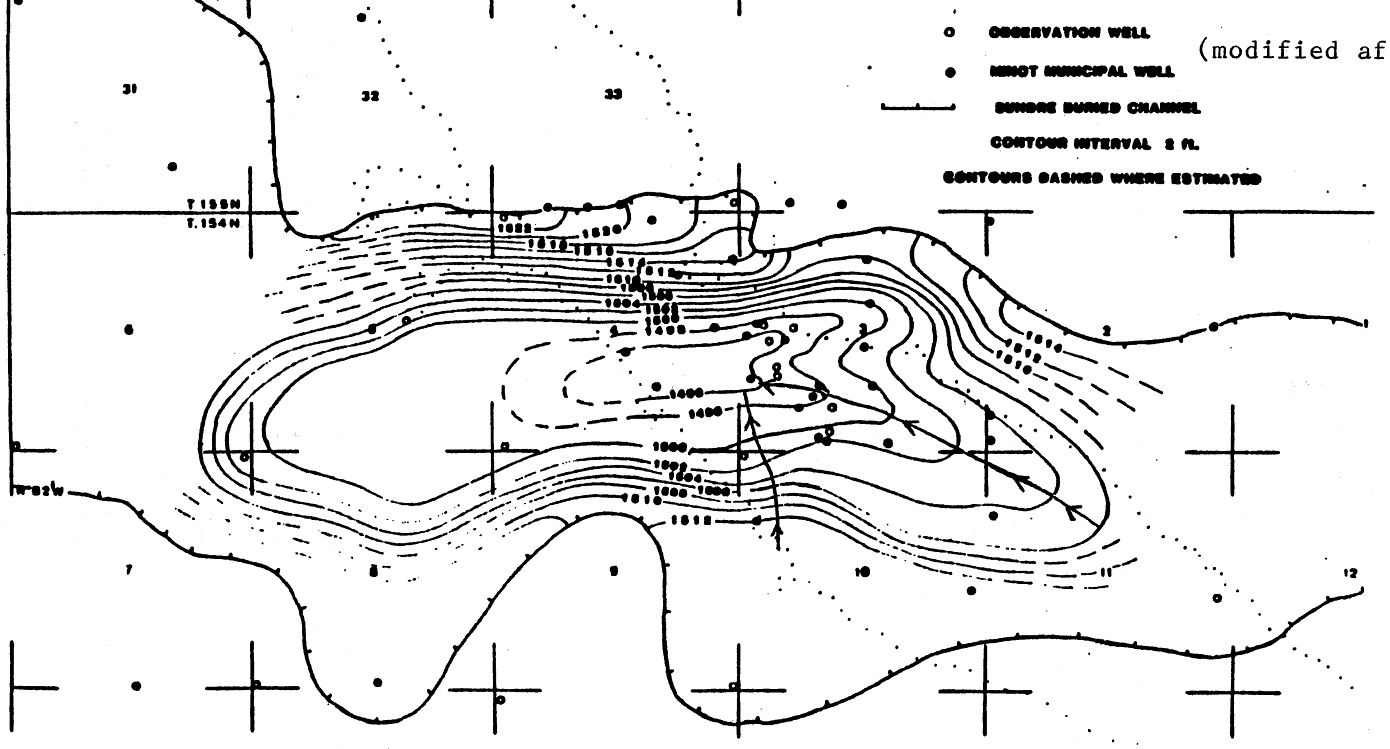
SUNDRE WATER LEVELS: NOV. 1978

(modified after Poore,1987)



SUNDRE WATER LEVELS: DEC. 1982

(modified after Poore,1987)



SUNDRE WATER LEVELS: AUG. 1985

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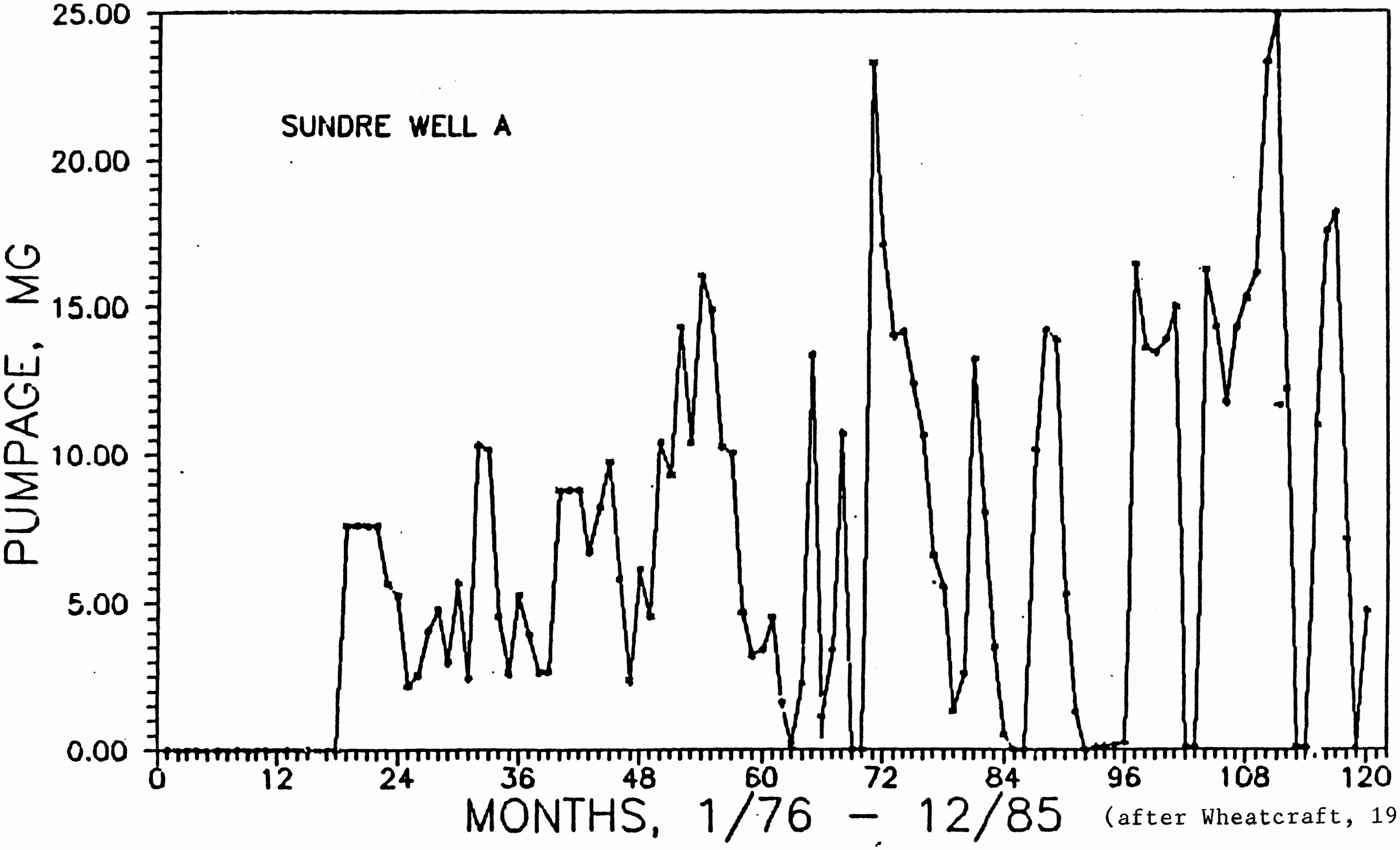
APPENDIX C

PUMP RATES FOR WELLS A-E



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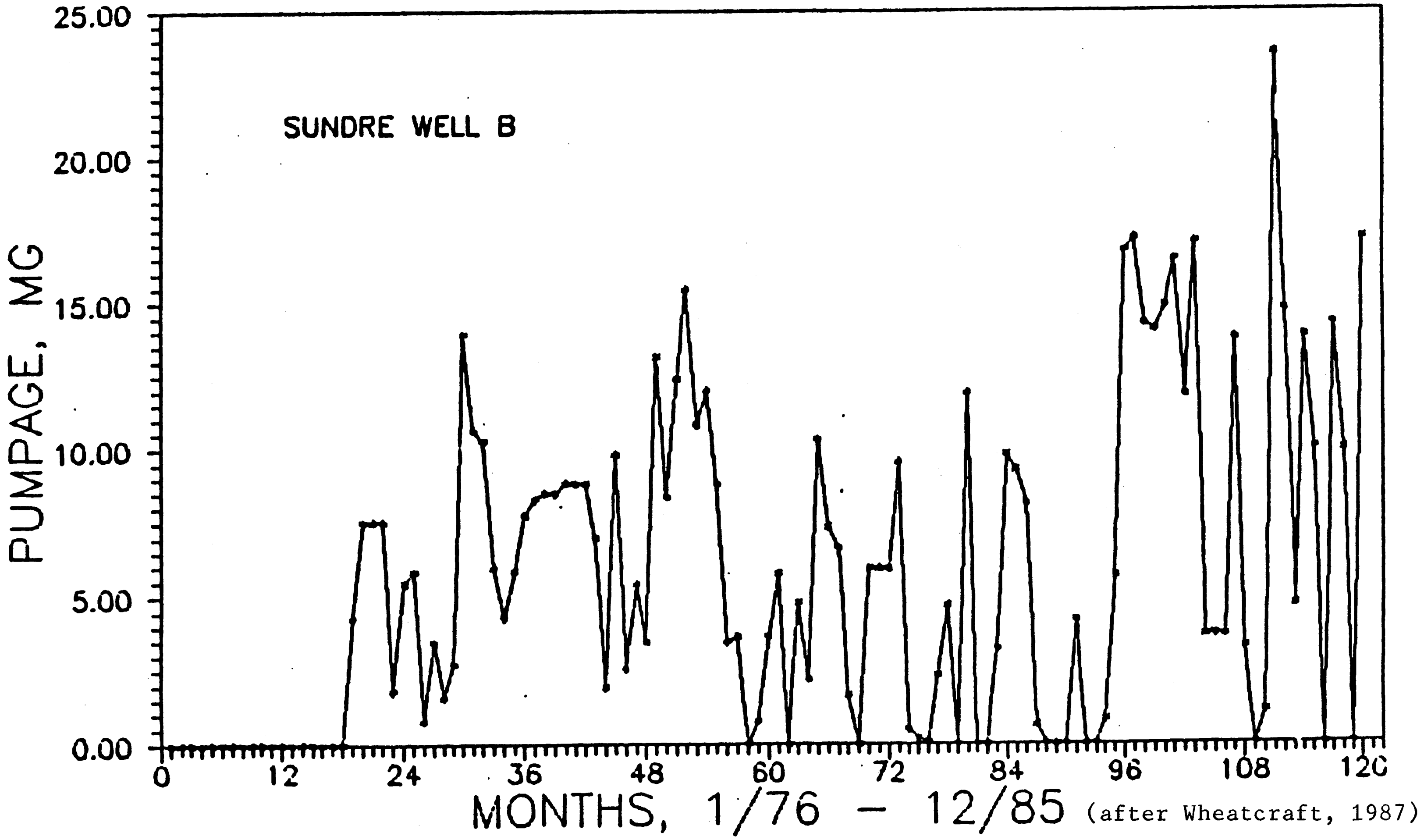

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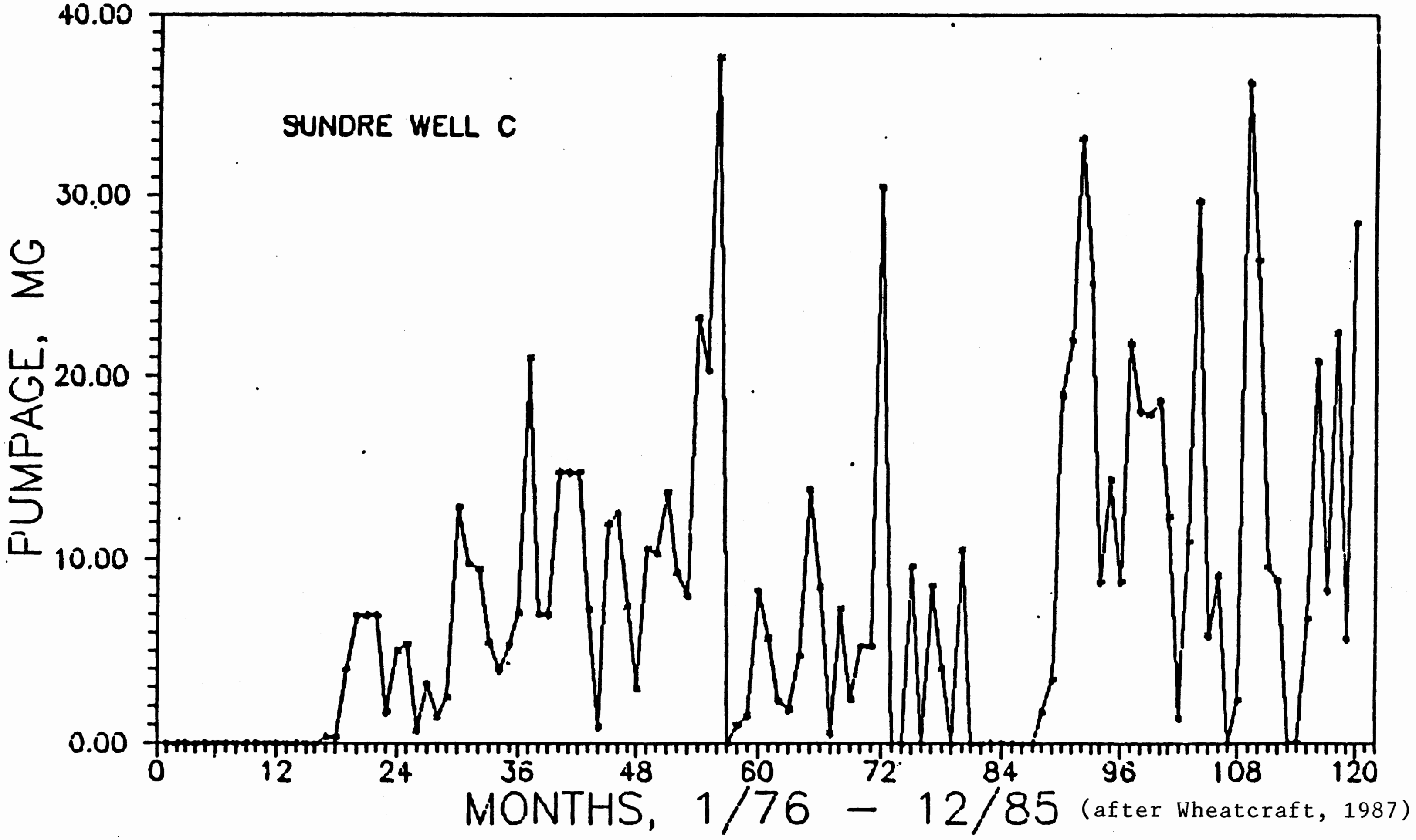

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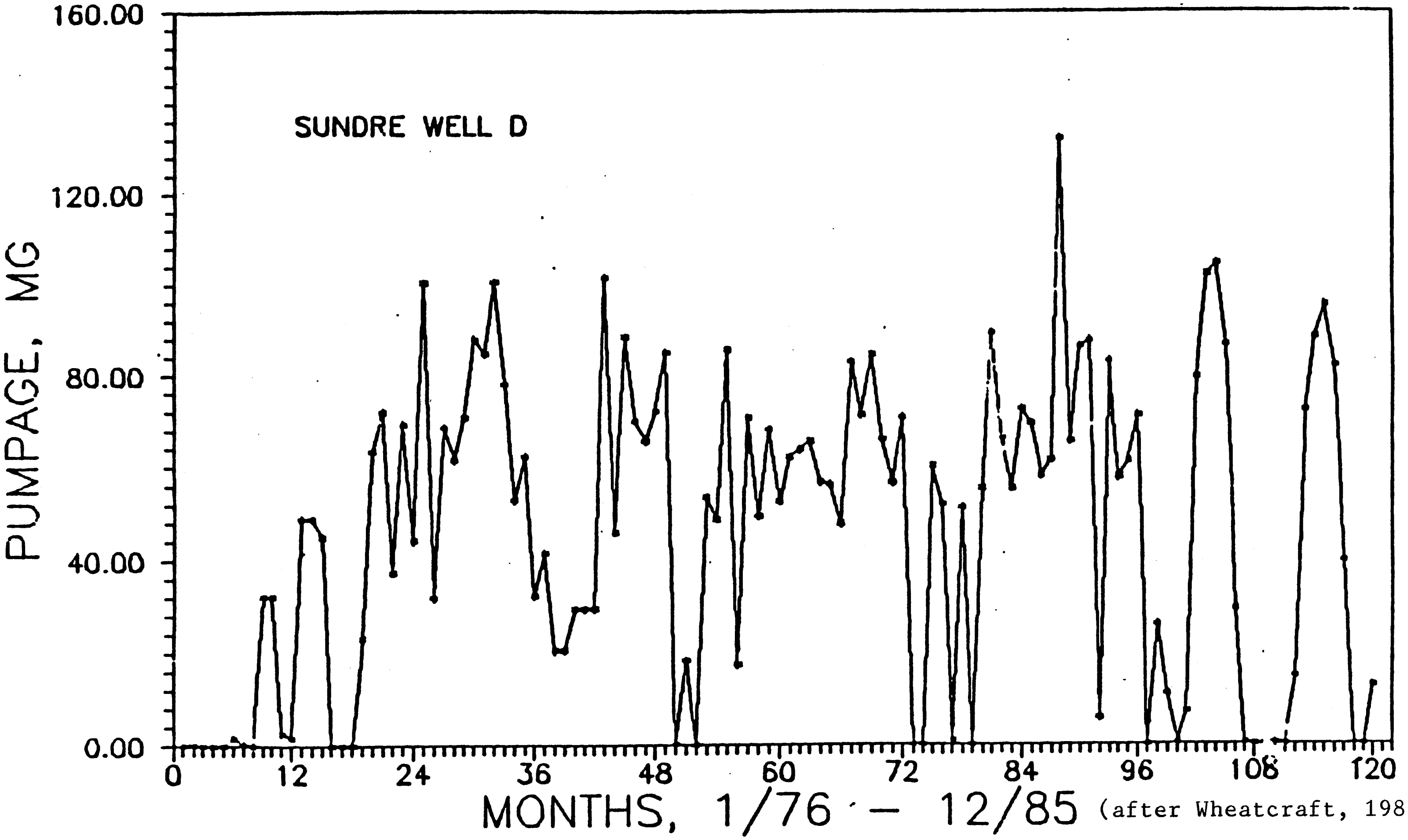

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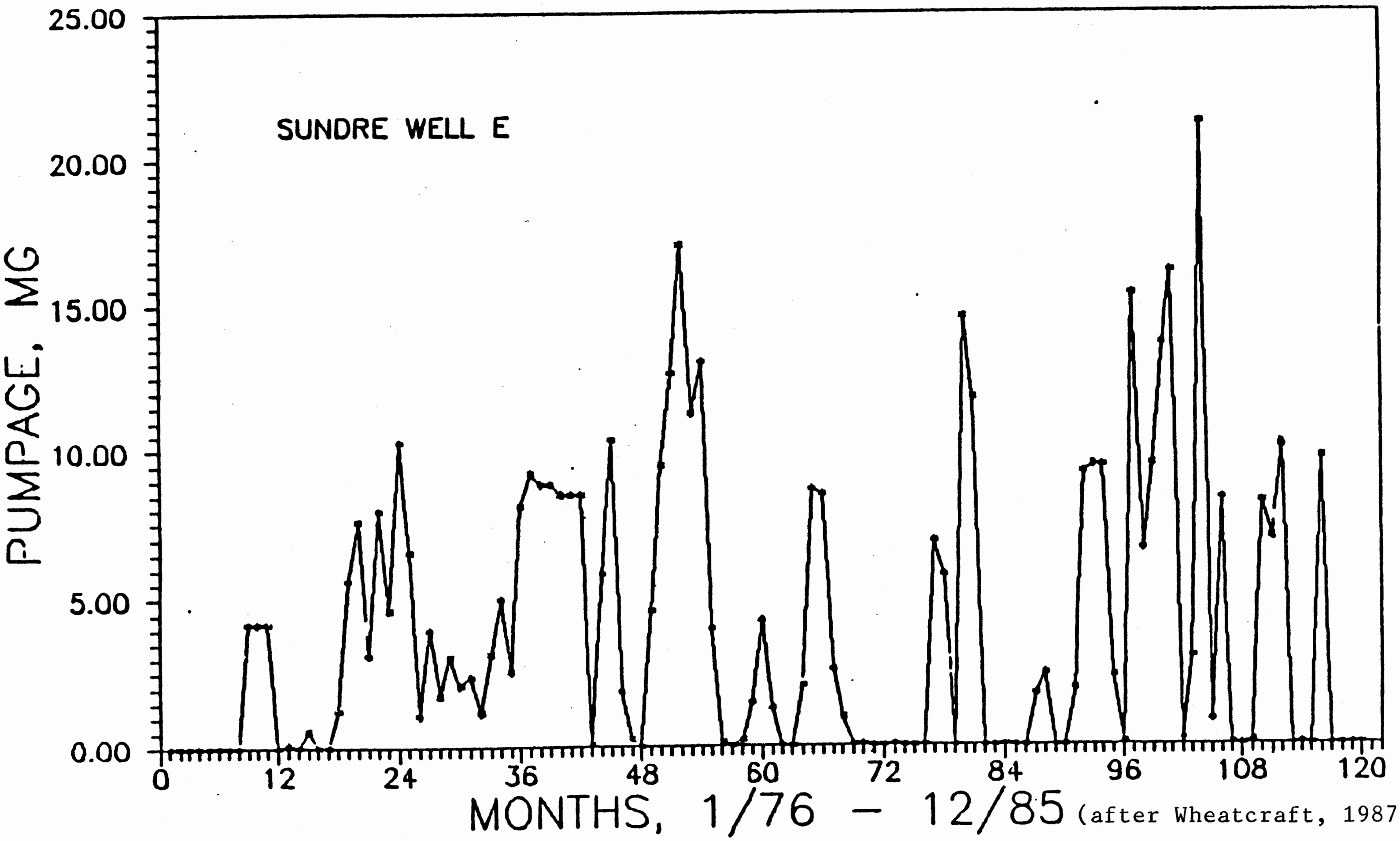

(after Wheatcraft, 1987)

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