DIGITAL SIMULATION OF THE REGIONAL EFFECTS OF SUBSURFACE INJECTION OF LIQUID WASTE NEAR PENSACOLA, FLORIDA

By Michael L. Merritt

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CONVERSION FACTORS

For readers who may prefer to use metric units rather than inch-pound units for the terms used in this report, the following conversion table is provided:

Multiply inch-pound unit	By	To obtain metric unit
foot (ft)	0.3048	meter (m)
mile (mi)	1.609	kilometer (km)
square mile (mi^2)	2.590	square kilometer (km^2)
cubic foot per second (ft^3/s)	0.02832	cubic meter per second (m^3/s)
pound per cubic foot (lb/ft^3)	16.02	kilogram per cubic meter (kgm/m^3)
pound-force per square inch (lb/in^2)	6.895	kilopascal (kPa)
cubic foot per day (ft^3/d)	0.02832	cubic meter per day (m^3/d)
gallon per minute (gal/min)	0.06309	liter per second (L/s)

* * * * * * * * * * * * *

National Geodetic Vertical Datum of 1929 (NGVD of 1929).--A geodetic datum derived from a general adjustment of the first-order level nets of both the United States and Canada called NGVD of 1929 is referred to as sea level in this report.

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ABSTRACT

Industrial, organic, liquid waste has been injected into a permeable part of the lower limestone of the Floridan aquifer at one site since 1963 and at another site since 1975, raising water levels in the injection zone throughout a large region in northwestern Florida. Data from the injection operations have made possible the application of a computerized mathematical model for a simulation of injection effects in the region.

The hydrogeologic conceptual model of the injection zone is that of limestone rocks of moderate permeability hydraulically isolated from the overlying upper limestone of the Floridan aquifer by a thick layer of clay and in which hydraulic conductivity decreases rapidly below the upper 60 feet. To the north, the overlying confining layer crops out and the unconfined injection zone is at or near land surface. To the east, the confining layer pinches out and the undifferentiated Floridan aquifer is overlain by coarse clastics. The injection zone appears to be bounded laterally by permeability barriers to the northwest and west due to facies changes and faults. There is some evidence for a permeability barrier to the southwest caused by the pinching out of the upper, transmissive part of the injection zone, and to the south there is likely an interface with saltwater near the presumed subcrop of the injection zone in the Gulf of Mexico.

Measured and reconstructed preinjection water levels suggested that flow in the aquifer was from the northern recharge areas toward the southeast. A steady-state model simulation incorporating the cited boundary assumptions approximately simulated this pattern. The U.S. Geological Survey Water-Resources Division two-dimensional flow model and the subsurface waste injection program (SWIP) were calibrated to simulate the water-level rises at various monitor wells since 1963. Transmissivity values ranging from 850 feet squared per day to 4,000 feet squared per day and a storage coefficient of 2.75×10^{-4} were used. Sensitivity analyses showed that computed water-level changes deviated appreciably from calibrated values in response to moderate changes in either transmissivity or storage parameter specifications.

The predictive use of the calibrated model of water-level changes is understood to be restricted to the geographical locations of data used for calibration, and the model of the regional flow system is considered to be highly generalized. The latter was a basis for rough estimates of travel times of injected waste and adjacent saline water to locations of regional hydrologic significance. In attempts to incorporate transport calculations

into the regional hydraulic model, numerical dispersion introduced by the large time and spatial discretizations required by the scale of the problem was far greater in degree than the hydrodynamic dispersion directly entered into the model as a best estimate of that occurring in the aquifer, making this simulation approach infeasible.

INTRODUCTION

The increasing scope of man's industrial activities and the consequent need to dispose of wastes has led to innovative technologies such as subsurface injection of wastewaters into aquifers containing water considered unusable for other purposes. Such has been the means used since 1963 at injection site 1 and since 1975 injection site 2 by two companies disposing of liquid waste from the manufacturing of chemicals at their plants near Pensacola in the western panhandle of Florida (fig. 1).

Waste injection at these and other sites has led to concern that aquifers containing potable water could become contaminated, motivating studies of the chemical, hydraulic, and thermal effects of injection. The local and regional effects of the western Florida operations are some of the more extensively studied in the United States, as part of a U.S. Geological Survey nationwide research program. The local program of data collection and interpretive study has been conducted in cooperation with the Florida Department of Environmental Regulation and with the support of the owners of the injection systems.

The U.S. Geological Survey sponsored the development of a computerized mathematical model (SWIP) for simulation of waste injection effects (INTERCOMP Resource Development and Engineering, Inc., 1976). The use of computer models contains the potential to make predictions concerning future pressure increases in injection zones and the movement of injected waste and native waters, thereby providing guidance for water-management decisions. Data from the western Florida injection operations made possible the use of SWIP in a field study.

The model analyses were conducted as a part of the Federal study in which the State provided special matching funds, obtained partly from the chemical companies, for the specific purpose of applying the SWIP model. Potential results were understood to encompass simulation of hydraulic effects and the transport of injected waste and native saline water and the use of these simulations for interpretations considered to have hydrologic and water-management significance. Not all of the anticipated results were fully achieved, but worthwhile products emerged from the principal lines of endeavor: (1) simulation of the regional flow system; (2) simulation of observed injection-zone water-level changes at various observation wells; and (3) incorporation of a waste transport simulation into a regional hydraulic model. The documentation of the analyses and problems encountered will be useful guidance in planning further investigations with similar objectives.

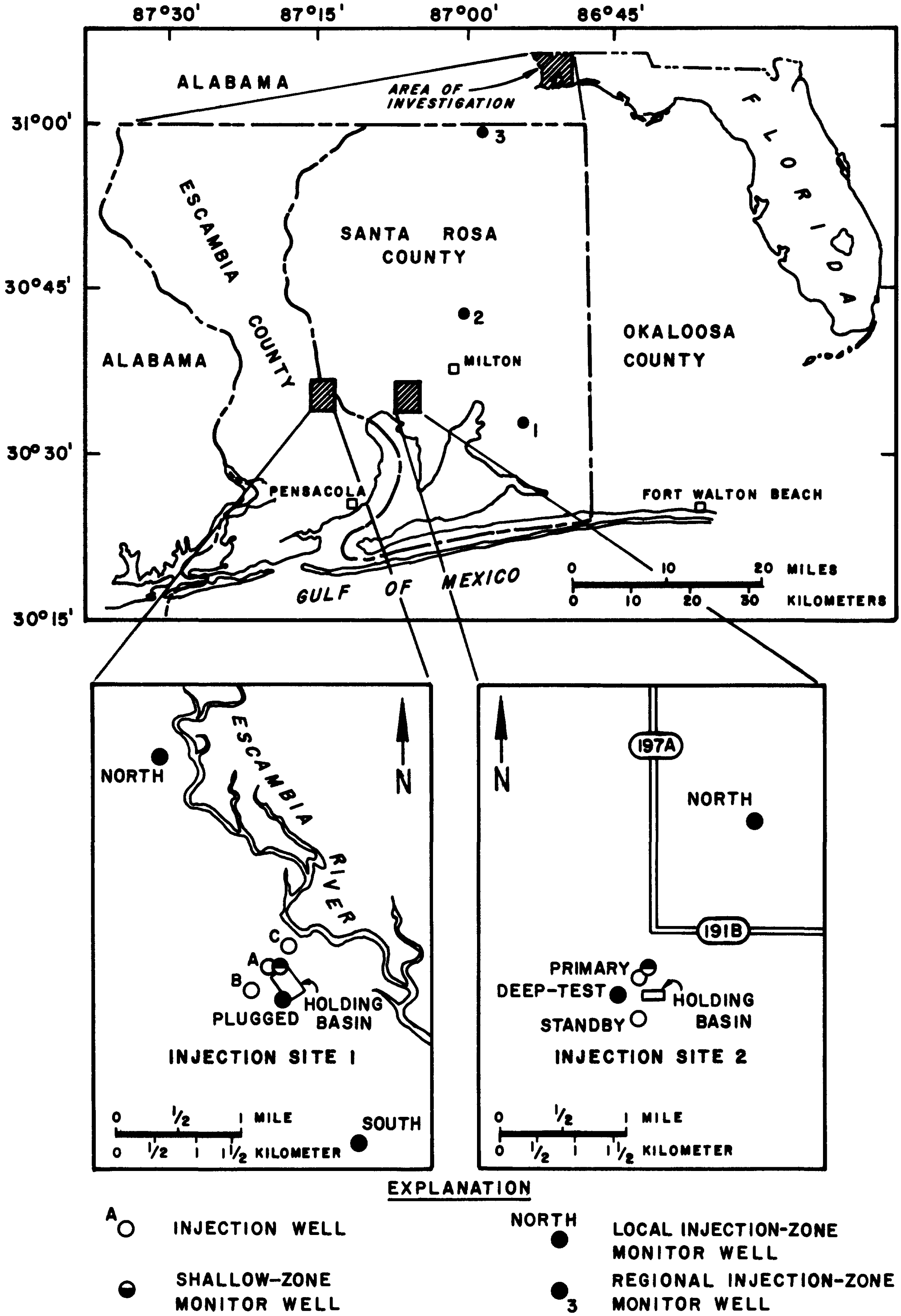

Figure 1.--The injection sites and regional monitor wells 1, 2, and 3.

Purpose and Scope

The purpose of this report is to document the methodology used and significant results achieved in the course of efforts directed along the three previously cited lines of endeavor: (1) The generalized simulation of the regional flow system; (2) the simulation of observed water-level changes; and (3) incorporation of transport calculations into the regional flow model.

To accomplish the first objective, the hydrogeology of the study area was considered for the purpose of constructing a conceptual model of the injection zone and its boundaries. As the hydrology of hydrostratigraphic units such as the lower limestone of the Floridan aquifer has not been documented in much detail, this required interpretation and correlation of results of various other areal and site-specific studies. The first and second objectives also required consideration of the hydraulic effects of the presumed natural boundaries of the injection-zone flow system. The influence of the boundaries is elucidated by the description of several steps in the construction of the hydraulic model: (1) the initial version which assumed no boundaries existed, (2) use of image-well analyses to individually test the hydraulic effect of each boundary, and (3) incorporation of all boundaries into the final flow model.

The input parameters required for transfer of the hydraulic solution to SWIP are described, as are the numerical problems encountered while trying to compute waste transport. As SWIP has not been widely used, it is briefly described, and a parallel description of the two-dimensional flow model used in early stages of the hydraulic analysis is included to facilitate comparison.

The scope of the report thus encompasses brief model descriptions, a development of regional hydrogeology, description of several steps in the construction of the hydraulic model and interpretation of results, and a discussion of problems associated with the transport simulation. The study area (fig. 1) was that part of northwestern Florida in which subsurface hydraulic effects of injection are manifest. These effects are most appreciable in south-central Escambia and Santa Rosa Counties, where the two injection sites are located. A much larger section of the aquifer, underlying parts of Alabama, Okaloosa and Walton Counties in Florida, and the Gulf of Mexico, was included in the area of the models in order to incorporate natural hydrologic boundaries.

The anticipated audience for the report includes those interested in its conclusions of water-management significance related to the practice of waste injection in northwestern Florida as well as those more generally interested in the approach to a field study of injection into a confined aquifer, a study of which the principal features were the limited data base and the application of a relatively new and sophisticated computer model. Neither the theoretical basis nor the methodology of the study are considered to be of major research significance. However, evaluation of the conclusions of the study will require review of its methodology by concerned agencies. Thus, the technical level of the writing is aimed at individuals with some degree of experience with the use of computer models in field studies; the discussion is straightforward, carefully based upon fundamental principles, and stresses the practical results of each step.

Acknowledgments

The U.S. Geological Survey wishes to express its appreciation of the support and cooperation of the Monsanto Company and the American Cyanamid Company for data collection and interpretive efforts which supported the numerical model analysis and for their support of the present study.

John Vecchioli, U.S. Geological Survey, Tallahassee, Fla., proposed the digital model analysis with SWIP as a new initiative in the program of waste injection studies in Florida, and provided the author with guidance and training. C. A. (Jerry) Pascale, U.S. Geological Survey, Tuscaloosa, Ala., leading the investigation into effects of the western Florida injection operations, made various data available and provided general expertise concerning the hydrogeology of northwest Florida. The author is indebted to their current (1983) counterparts, John J. Hickey, U.S. Geological Survey, Tampa, Fla., and Bernard J. Franks, U.S. Geological Survey, Tallahassee, Fla., for their efforts to support finalization of the report of the study. The author is grateful to Michael Planert, U.S. Geological Survey, Tuscaloosa, Ala., for an exceptionally thorough technical review.

The author would also like to express appreciation to James W. Mercer and Charles R. Faust, formerly with the U.S. Geological Survey, Reston, Va., for their introductory course and subsequent help in the use of SWIP, and to Steven P. Larson, formerly with the U.S. Geological Survey, Reston, for additional help.

THE INJECTION SYSTEMS AND MONITORING PROGRAMS

Injection Site 1

The assessment of the geology of Escambia and Santa Rosa Counties by Marsh (1966), supported by an assessment of the water resources of the two counties (Musgrove and others, 1961 and 1965), indicated the environmental feasibility of subsurface waste injection into the lower part of the Floridan aquifer. After tests at a well constructed by the Monsanto Company in 1963 (well A, fig. 1) verified the economic feasibility of injecting wastes, the company began to do so on a continual basis. The hydrogeologic setting and the development of the system are described by Barraclough (1966); Goolsby (1971); Foster and Goolsby (1972); Faulkner and Pascale (1975); and Pascale and Martin (1978). A comprehensive summary of hydraulic, geologic, and water-quality data is provided by Hull and Martin (1982).

Since governmental agencies required a monitoring program, two monitor wells were drilled in 1963. The "shallow-zone" monitor was 100 feet from the injection well and open to the upper part of the Floridan just above the Bucatunna Clay member of the Byram Formation, a confining layer, for the purpose of detecting upward leakage of waste from the injection zone. The other ("plugged," fig. 1) was open to the injection zone about 1,300 feet south of the injection well for the purpose of monitoring hydraulic and geochemical effects. In 1964, a second injection well was drilled about 1,300 feet from the first (well B, fig. 1) and wastewater was injected alternately, or concurrently during heavy rainfall periods, in wells A and B (C. G. Hoffman, Monsanto Company, written commun., 1983). In 1982, a third injection well (well C, fig. 1) was completed, as well as a second shallow-zone monitor well (not illustrated).

The acidic waste fluid is kept in outdoor holding ponds for several days prior to injection. Thus, its temperature when injected tends to vary seasonally. Its viscosity is nearly the same as for pure water, and its density was measured to be 62.71 lb/ft^3 at atmospheric pressure (laboratory temperature not recorded) in May 1977 (C. A. Pascale, oral commun, 1977).

At first, the waste was treated with aqueous ammonia to raise the pH to about 5.5 before injection. In May 1964, 10 months after injection began, chemical analyses indicated that the treated waste had reached the vicinity of the injection zone monitor well. In April 1968, the treatment was halted and in January 1969 acid waste with a pH of about 2.3-3.0 was detected at the monitor well. The possibility of corrosion of the well casing and release of acid waste to overlying aquifer units led to plugging of the monitor well in February 1969. In response to the consequent lack of monitoring within the injection zone, the south and north deep monitor wells (fig. 1) were constructed in late 1969 and early 1970. The south monitor is 1.5 miles south-southeast of the injection site, and the north monitor 1.9 miles north-northwest of the site.

Injection rate data have been made available by the Monsanto Company as daily averages in gallons per minute for the entire period of injection, except for 4 months in 1963. The combined monthly average rate for the two injection wells until 1978, when the active phase of this investigation was completed, is shown in figure 2A. This rate varied from a low of 550 gal/min in 1963 to a high of 2,605 gal/min in 1972. The average injection rate in the years 1981-83 was appreciably less than in preceding years (about 1,300 gal/min). The cumulative increase of the volume of fluid injected since 1963 and until 1978 is shown in figure 2B. By March 1978, 14.7×10^9 gallons had been injected. The injection pressure at the wellheads has not varied linearly with the injection rate, as the acidic waste has gradually dissolved the limestone about the wells, locally increasing the porosity and transmissivity. Thus, the wellhead pressure has been observed to drop even while the rate of injection increased (Faulkner and Pascale, 1975).

Pressure data were obtained from the first deep monitor well before it was plugged. Wellhead (land-surface) pressure data have been recorded continuously, beginning with well completion, at the south and north deep monitor wells, and values for every fifth or last day of the month are converted and tabulated as water levels. The injection of waste has caused (pressure-equivalent) water levels to rise as much as 235 feet in 1978 at the north and south monitor wells and to rise appreciably even at great distances (about 30 feet by 1978 at a monitor well 22 miles away). Water levels at nearby monitor wells did not show a continual rise; water levels fell when average injection rates were consistently low for several successive months.

Pascale and Martin (1978) describe an increase in bicarbonate and dissolved organic carbon at the south monitor well beginning in September 1973 that indicated the arrival of traces of the injected waste. The concentration of the injected waste at the monitor well could not be measured precisely, however, due to the absence of any known conservative tracer.

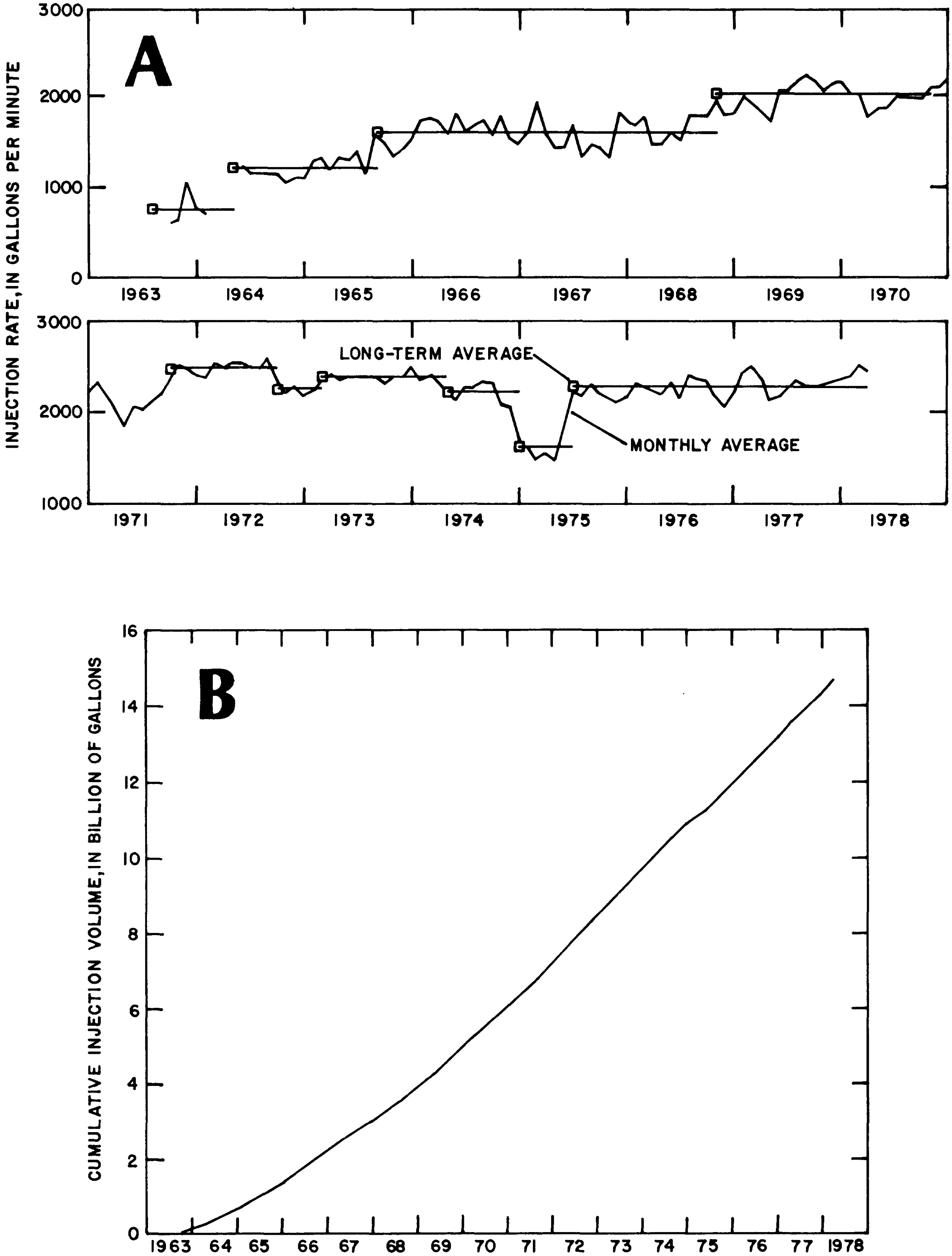

Figure 2.--(A) - Injection rates and (B) - the cumulative increase of injection volume at injection site 1.

Regional Monitor Wells

In order to evaluate the regional effects of injection at site 1, the U.S. Geological Survey constructed two monitor wells open to the injection zone at locations relatively distant from both injection sites (fig. 1). Regional monitor well 1 is 22 miles east-southeast and regional monitor well 2 is 17 miles northeast of injection site 1 (Pascale, 1976). Both were completed in January 1974. Water levels at these two monitor wells, recorded continuously from time of well completion through the period of the study, have continued to rise, though remaining below or just above land surface. This showed the effects of Monsanto Company waste injection and the later additional influence of the American Cyanamid Company waste injection. Data obtained during and since well construction are included in the summary by Hull and Martin (1982).

A damaged supply well near the Alabama-Florida border, and about 35 miles northeast of the injection sites, was repaired for use as a distant monitor of the injection systems (regional monitor well 3, fig. 1). It provided a few water-level data between mid-1966 and mid-1969, and a few more after early 1974, measured by tape down to water.

Injection Site 2

The American Cyanamid Company operates an acrylic fiber plant near Milton, Fla. Some manufacturing processes at the plant produce strong organic wastes (Ehrlich and others, 1979) that require an appropriate method for their disposal. The deep test monitor well was constructed in 1971 for the purpose of determining the feasibility of injecting the liquid waste at the site (injection site 2, fig. 1). The well casing was later perforated and opened to the upper part of the injection zone and began to serve a dual purpose as a distant monitor of the effects of waste injection at site 1, about 8 miles to the west-northwest, and as a facility for further testing by the company.

In 1975, several years after tests established the feasibility of waste injection, a pair of injection wells were constructed nearby (Pascale, 1975). The deep test monitor well was then 1,025 feet southwest of the new primary injection well, and the standby injection well 1,560 feet south of the primary injection well (fig. 1). Waste injection began at the primary well, and the standby well and deep test monitor well were used as monitors. A more distant injection-zone monitor well, 1.55 miles northeast of the primary injection well, was also completed in 1975. A shallow monitor well was drilled into the upper part of the Floridan so that any leakage through the confining bed could be detected by its effect upon the water level and water quality at its location, 28 feet from the primary injection well. Hydraulic, geologic, and chemical data collected during and after well construction are described by Pascale and Martin (1977), and are included in the data summary of Hull and Martin (1982).

Injection rate data have been made available by the American Cyanamid Company as daily averages in gallons per minute for the entire period of injection. The monthly average injection rates are shown in figure 3A. These rates have varied from 350 gal/min to 660 gal/min, but the long-term average (550 gal/min) has not varied much from its value after the first several months. Figure 3B shows the cumulative increase of the volume of fluid injected from June 1975 until June 1978, when 0.89×10^9 gallons had been injected. Pressure at the wellhead has been recorded continuously, beginning with completion of well construction, at the standby injection well and at the monitor wells. The maximum value every fifth and end-of-month day is converted to a water level for a tabular summary.

The waste fluid contains a conservative tracer, sodium thiocyanate (NaSCN). Waste fluid viscosity is nearly the same as for pure water and its density was measured to be 62.52 lb/ft^3 in March 1977 (C. A. Pascale, oral commun., 1977). The fluid is placed in a small holding pond for hours or days prior to injection and is aerated by mixing to promote primary treatment. The acidic waste is neutralized with sodium hydroxide and treated with alum prior to injection (Ehrlich and others, 1979). The neutralized waste fluid was believed not to have appreciably dissolved limestone about the well in the injection zone (C. A. Pascale, oral commun., 1977).

In February 1976, increases in bicarbonate and dissolved organic carbon concentrations, as well as traces of thiocyanate, were detected at the deep monitor well (Ehrlich and others, 1979). In December 1976, the thiocyanate concentration at the deep monitor well was 50 percent of the average concentration in the injected fluid. By November 1977, the concentration at the well was nearly 100 percent of the injected concentration. Beginning April 1976, thiocyanate and the other chemical traces of the waste fluid were detected at the standby injection well. The thiocyanate concentration in September 1978 was between 39 and 51 percent of the injected fluid concentration at the standby injection well.

HYDROGEOLOGIC CONCEPTUAL MODEL OF THE STUDY AREA

A stratigraphic description of the geology of the study area to a depth of 2,800 feet is provided by Marsh (1966). Geologic sections parallel and normal to the regional dip (figs. 4 and 5) show the major stratigraphic divisions. Additional interpretation is provided by Puri and others (1973) and Faulkner and Pascale (1975). Detailed stratigraphy at injection site 1 was revealed by lithologic data collected during construction of the first injection well (Barraclough, 1966) and during construction of the north and south deep monitor wells (Foster and Goolsby, 1972). Lithologic logs also provided data at injection site 2 (Pascale, 1975; Ehrlich and others, 1979) and at the regional monitor wells (Pascale, 1976). Hull and Martin (1982) summarize the data.

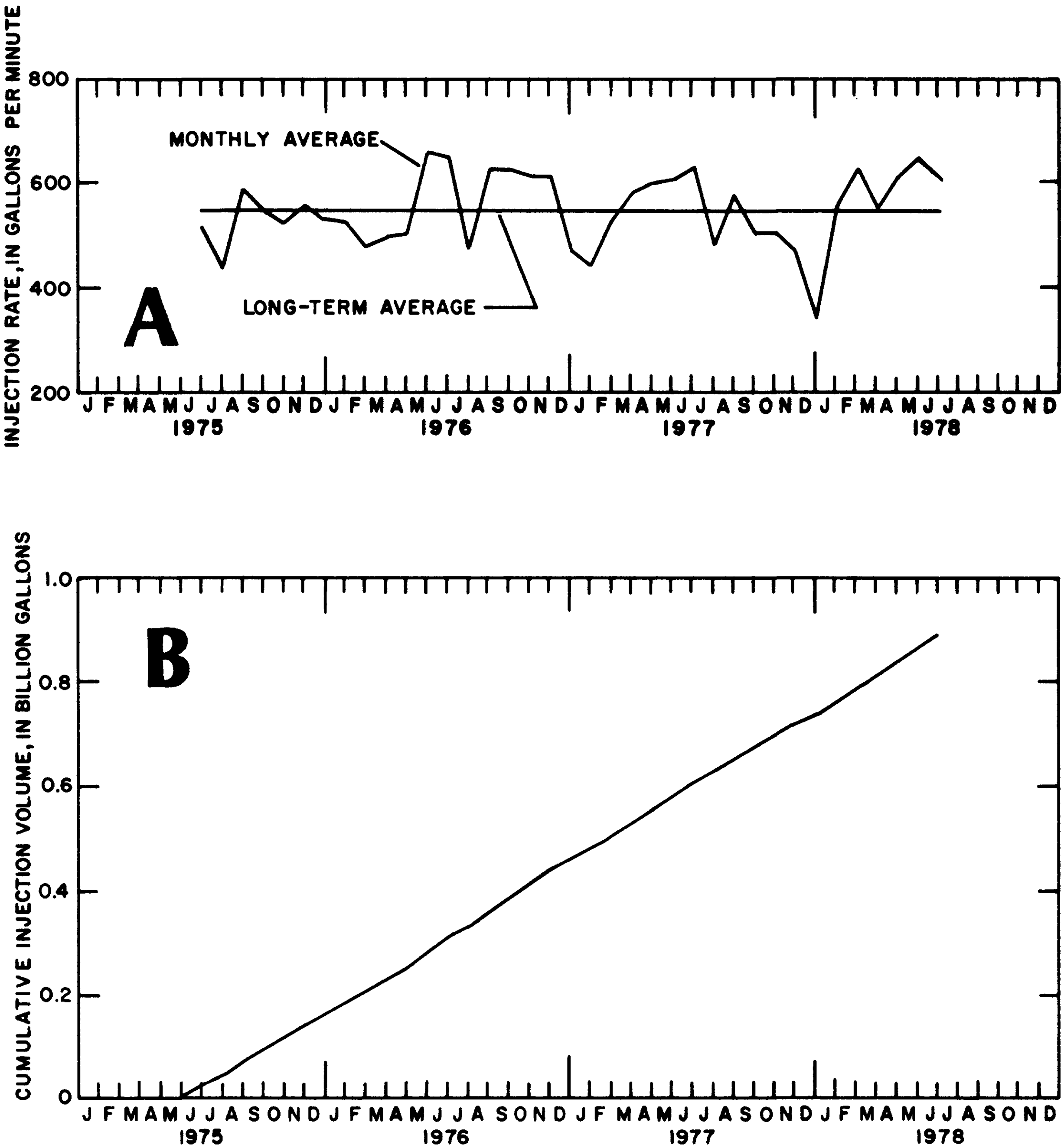

Figure 3.--(A) - Injection rates and (B) - the cumulative increase of injection volume at injection site 2.

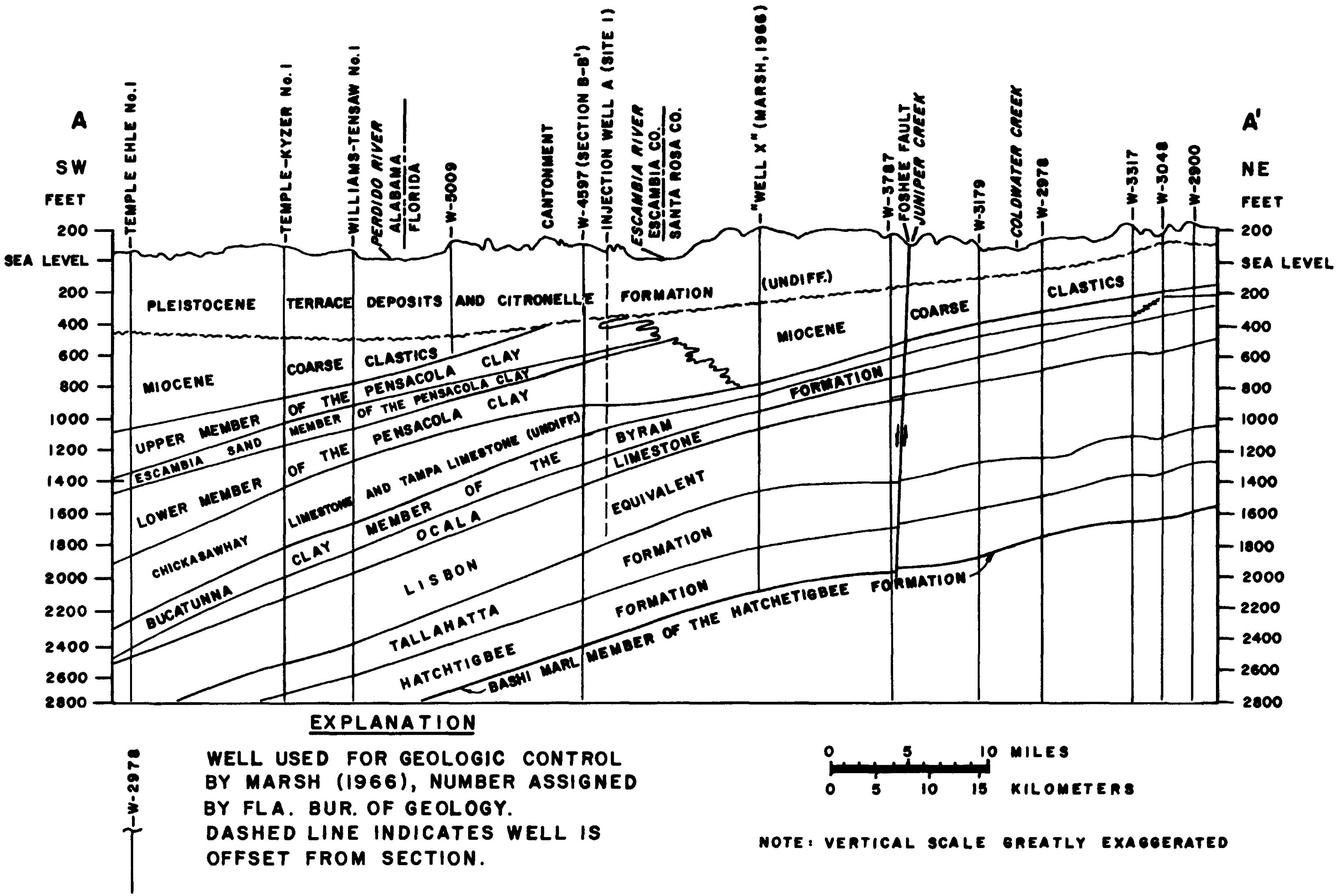

Figure 4.--Geologic section A-A' across Escambia and Santa Rosa Counties parallel to the regional dip (see fig. 6). (Modified from Marsh, 1966, fig. 6.)

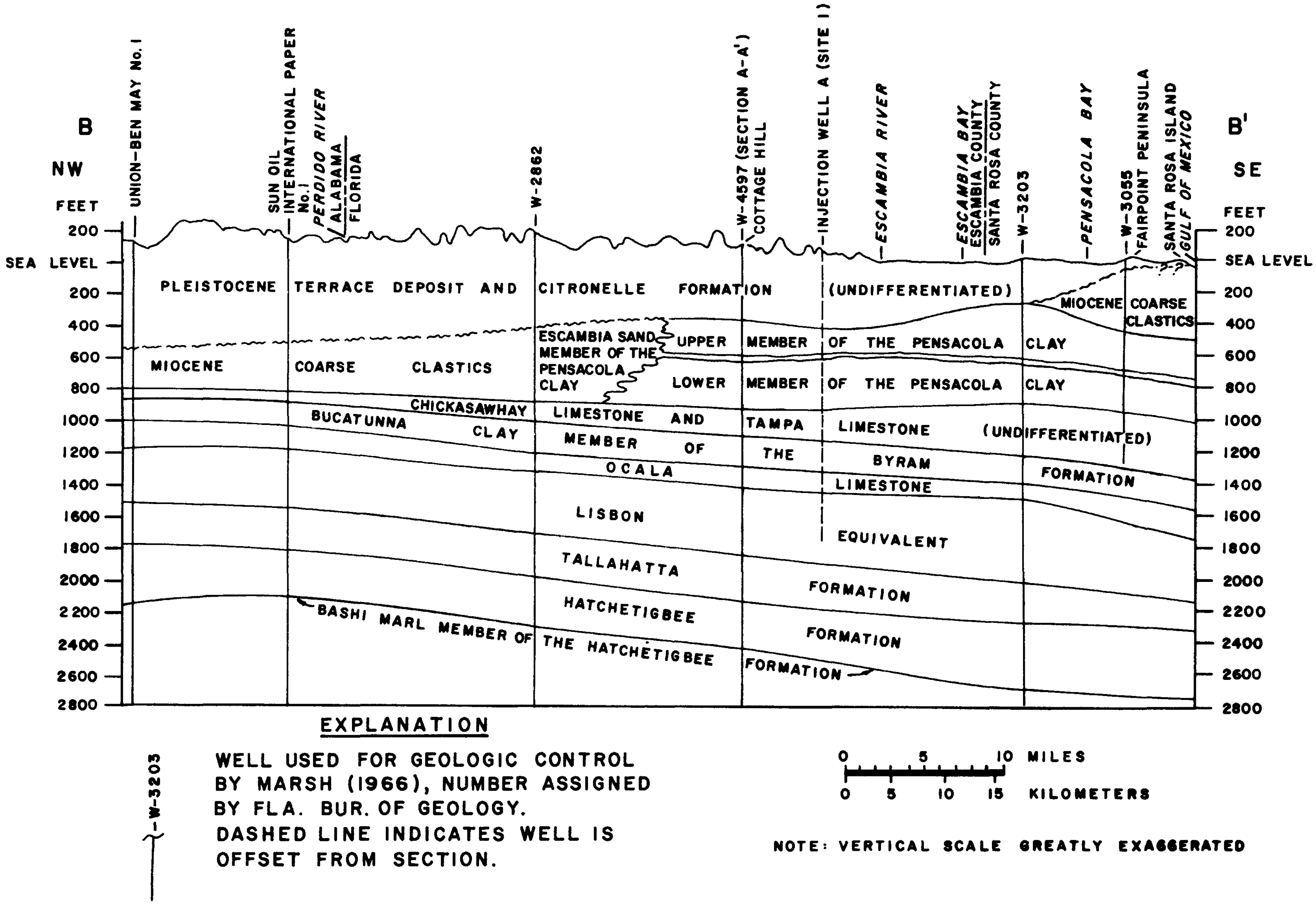

Figure 5.--Geologic section B-B' across Escambia and Santa Rosa Counties parallel to the regional strike (see fig. 6). (Modified from Marsh, 1966, fig. 8.)

The geologic section A-A'(fig. 4) shows the formations that underlie the surficial layers of clastics dipping toward the southwest, with the slope of the dip increasing in that direction. Well logs from the various wells drilled in connection with two waste injection programs show good agreement with contours on the top of the Ocala Limestone shown by Marsh (1966). The Ocala Limestone (of late Eocene age) is the upper part of the lower limestone of the Floridan aquifer. The underlying formation, the equivalent of the Lisbon (Marsh, 1966), also consists primarily of limestone and is included in the lower Floridan (Trapp and others, 1977). Injection well A at injection site 1 is open to the entire interval of the Ocala and to part of the Lisbon equivalent, but nearly all flow occurs within the upper 100 feet of the open interval, as it also does at injection site 2. Thus, the injection zone is identified as permeable strata within the upper 100 feet, entirely within the Ocala Limestone and underlain by much less permeable limestone at the injection sites and possibly throughout the entire study area.

The relative areal extents of continuous sections of the various geologic units overlying the Ocala Limestone (fig. 6) are of considerable importance in that they determine hydraulic conditions which control the pattern of regional flow and affect response to hydraulic stress. The limits of these aquifers and confining layers are pinchouts, undersea or land-surface outcrops, or structural or lithologic discontinuities (faults or facies changes). A preliminary delineation of formation limits related to the investigation was made by J. A. Miller (written commun., 1977) and was based upon published U. S. Geological Survey areal studies and lithologic and geophysical logs from oil test wells. The positions of some of the boundaries are inferred on the basis of limited data, as indicated by dashed lines in figure 6.

More than 400 feet of surficial clastic sediments of Pleistocene through Miocene age comprising the sand-and-gravel aquifer, the principal source of freshwater in Escambia and Santa Rosa Counties, overlie several hundred feet of mixed sand and clay which comprise the upper and lower members of the Pensacola Clay (Florida Bureau of Geology terminology, used by Marsh, 1966), of Miocene age. Both members confine underlying aquifers where the members are present. The northern and eastern limits of the upper member of the Pensacola Clay are in central Escambia County, Fla., and in west-central and southeastern Santa Rosa County (Marsh, 1966; Trapp and others, 1977). The lower member of the Pensacola Clay extends farther to the north and east than the upper member, north into central Escambia and Santa Rosa Counties and east into west-central and southeastern Okaloosa County (Marsh, 1966). The limits of both clays are facies changes, north and east of which deposits of the same age are composed of coarse clastics (sand and gravel). Where the more extensive lower member of the Pensacola Clay changes to coarse clastics, the underlying upper limestone of the Floridan aquifer is either unconfined or poorly confined. The clays probably subcrop under the Gulf of Mexico to the south, provided they extend for tens of miles in that direction.

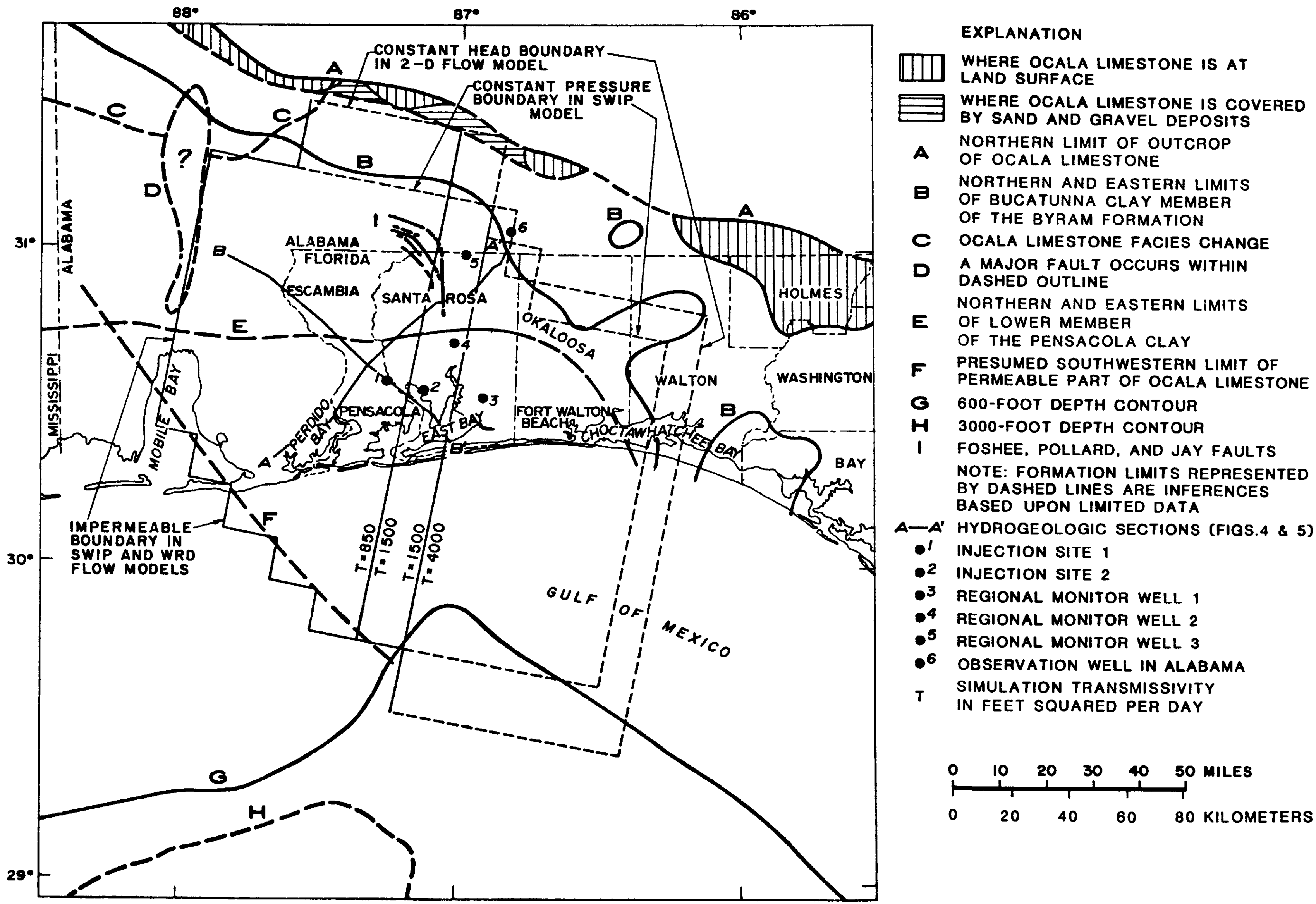

Figure 6.—Areal extent of geologic formations pertinent to study and correspondence with model boundaries. Compiled by J. A. Miller (written commun., 1977).

Though not shown in figure 6, the upper Floridan, described by Marsh (1966) as the Chickasawhay Limestone and Tampa Limestone (undifferentiated), crops out in southern Alabama well beyond the limit of the Pensacola clays (Cagle and Floyd, 1957); within the Florida Panhandle, the upper Floridan thickens to the south. To the east and west, the upper Floridan extends beyond the boundary of the area of investigation. In Walton County to the east, sections of Miocene clays may separate the Chickasawhay from the overlying Tampa, if these formations are analogous to the Suwannee Limestone and Chipola Formations of Pascale (1974). The formation is presumed to extend well into the Gulf of Mexico where, at sufficient depth, it would crop out. In the area of the injection sites, the upper Floridan is about 200 feet thick and contains water with chloride concentrations ranging from less than 100 to about 450 mg/L.

The upper and lower limestones of the Floridan aquifer are separated by the Bucatunna Clay Member of the Byram Formation, which extends northward towards its outcrop in Escambia County, Ala. (Cagle and Floyd, 1957), and eastward into Okaloosa, Walton, and Bay Counties, Fla. (Trapp and others, 1977). If both are continuous everywhere towards their northern outcrops, the Bucatunna Clay member would extend beyond the limit of the upper Floridan. However, a different situation prevails toward the east. The eastern limit, nearly 40 miles from injection site 2, is apparently an irregular pinching out of the Bucatunna beyond which the upper and lower Floridan are in contact. Isolated sections of clay may be present here and there, but detailed definition awaits further study.

The eastern limit of the Bucatunna Clay member apparently lies well beyond the limit of the lower member of the Pensacola Clay. This means that, where there are no isolated sections of the Bucatunna, the Floridan aquifer (undifferentiated) is unconfined, or poorly confined if thin sections of clay or marl suggested by Pascale (1974) and Trapp and others (1977) are present. Near Fort Walton Beach, upper Floridan water levels, in an area where the aquifer is confined by the lower member of the Pensacola Clay, have been greatly lowered by heavy withdrawals. This area is about 20 miles west of the estimated eastern limit of the Bucatunna Clay member underlying the upper Floridan. Thus, any propagation of upper Floridan drawdown effects from Fort Walton Beach pumping into the lower Floridan would originate at a point about 20 miles east of the source and about 45 miles east of injection site 2. The Bucatunna extends to the west beyond the boundary of the area of investigation. If the Bucatunna extends sufficiently far to the south, it crops out in the Gulf of Mexico.

Marsh (1966) shows the Bucatunna Clay member to be about 200 feet thick throughout most of Escambia and Santa Rosa Counties, thinning to 100-150 feet along the Florida-Alabama border. It attains its greatest thickness (220 feet) near injection site 1. The vertical hydraulic conductivity is low; values of approximately 2.6×10^{-7} to 2.9×10^{-6} ft/d were measured on cores from regional monitor wells 1 and 2 (Faulkner and Pascale, 1975). Together with the thickness of the layer, this makes the Bucatunna an effective confining bed for the underlying lower limestone of the Floridan aquifer. This is supported by water levels measured at monitor wells open to the lowest part of the upper Floridan just above the two injection systems. These water levels have not risen even though injection zone water levels locally have risen hundreds of feet.

Vertical faulting in an area centered on the Florida-Alabama border (fig. 6), which has resulted in the partial offset of the Bucatunna, is described by Marsh (1966). The estimated southernmost extent of the Foshee, Pollard, and Jay Faults is apparently about 15 to 20 miles north of the injection sites; the offset of the various formations at this point is negligible (fig. 4).

The northern outcrop of the Ocala Limestone, which is the principal part of the lower limestone of the Floridan aquifer and which includes the injection zone, is in southern Alabama, well beyond the northern limit of the Bucatunna Clay member. As surficial deposits north of the limit of the clay are primarily coarse clastics, lower limestone water levels are assumed to be nonartesian in southern Alabama. Where the Ocala Limestone and younger units comprising the upper Floridan are in contact beyond the eastern limit of the Bucatunna Clay member or Pensacola clays in parts of Okaloosa and Walton Counties and in other Florida counties farther to the east, water-table conditions are assumed, though possibly modified by lenses of sandy clay or low-permeability limestone. That water levels have declined more than 30 feet beyond the Bucatunna pinchout, apparently as the result of Fort Walton Beach pumping, suggests some degree of confinement. Stratigraphic data is unfortunately scanty. To the northwest, geologic samples show an Ocala Limestone facies change from sandy limestone to relatively impermeable materials which are principally clay (J. A. Miller, written commun., 1977).

To the west of the Florida Panhandle is a north-south oriented fault. According to J. A. Miller (oral commun., 1977), the degree of faulting is probably such that clays have been moved down opposite the Ocala Limestone, creating a permeability barrier. Geophysical logs of oil test wells (J. A. Miller, oral commun., 1977) show that approximately along a southeastward-directed line passing under Mobile Bay, there seems to be a pinchout of the upper part of the Ocala Limestone. Marsh (1966) shows the layer thinning to 50 feet or less in coastal Baldwin County, Ala. This may be a permeability barrier, as nearly all lateral water flow in the injection zone has been shown, at two isolated locations, to occur in the upper part of the Ocala Limestone. Figure 6 shows the 600-foot and 3,000-foot depth contours in the Gulf of Mexico between which would occur the southern outcrop of the Ocala Limestone if it extends that far with the same degree of dip. Marsh (1966) shows the top of the Ocala at about 1,600 feet on the Gulf Coast of Santa Rosa County.

Marsh (1966) also shows the Ocala Limestone to range from 90 to 235 feet in thickness within Escambia and Santa Rosa Counties, and to be about 150 feet thick at injection site 1. Cagle and Floyd (1957) show a thickness of 140 feet in eastern Escambia County, Ala., with a 60-foot lens of Yazoo Clay separating two 40-foot layers of limestone.

The equivalent of the Lisbon Formation, a thick layer of shaly limestone underneath the Ocala Limestone, is present throughout the area of investigation north of a probable Gulf of Mexico outcrop, as are the Tallahatta Formation, a layer of shale underneath the Lisbon, and the Hatchetigbee Formation, the next lower layer comprised primarily of clay.

The Injection Zone

Native Water Quality

Regional variations in the quality of the native water in the injection zone are of significance in that they aid efforts to interpret the regional flow system and to predict the regional and local movement of injected waste. Data are available from only five locations within the study area: the two injection sites and the three regional monitor wells. The data are summarized by Hull and Martin (1982), who refer to evolution of sampling techniques and stress that all water-quality analyses, particularly the earlier ones, must be qualified because of limitations inherent in the method of collecting samples from wells, particularly when appreciable stratification in quality occurs with depth within the aquifer. The analyses from the injection sites and regional monitor wells 1 and 2 include a vertical distribution of data collected soon after well construction.

Samples from the south and north monitor wells at injection site 1 (fig. 1), taken when the wells were allowed to flow during construction (Foster and Goolsby, 1972), showed chloride concentrations generally ranging from 6,000 to 8,000 mg/L (milligrams per liter) from 55 to 60 feet below the top of the formation, and generally about 10,000 mg/L from 160 to 180 feet lower. It is not known how chloride concentrations from levels above the casing bottom vary.

At injection site 2, about 8 miles to the east-southeast, chloride concentrations were measured at several wells in May 1975, before injection began. Concentrations 50 to 80 feet below the top of the lower limestone of the Floridan aquifer at the primary and standby injection wells were about 3,800 mg/L; about 200 feet below the top, they were about 9,000 mg/L. At the north deep monitor well, 1.55 miles to the northeast, the measured chloride concentrations ranged from 3,200 mg/L at the top of the lower limestone to 4,300 mg/L 170 feet lower.

In May 1977, about 12 miles further to the east-southeast, at regional monitor well 1, the chloride concentration 40 feet below the top of the lower limestone was 1,500 mg/L; 170 feet lower, the concentration was 5,300 mg/L. At regional monitor well 2, about 10 miles to the northeast of injection site 2, the chloride concentration was about 400 mg/L at both the top of the injection zone and 190 feet lower. Measured chloride concentrations at regional monitor well 3, about 28 miles to the northeast of the injection sites, were all less than 6 mg/L.

Because of the sparse areal distribution of data and qualifications related to collection methods, generalizations of the regional distribution of native water quality must be tentative. The indicated trend is increasing chloride concentration, together with vertical stratification, toward the southwest. Along the east-southeast transect from injection site 1 to regional monitor well 1, the chloride concentration apparently decreases though it remains stratified. From injection site 2 northeast to regional monitor well 2, the chloride concentration decreases to a level not much higher than that acceptable for public supply. At regional monitor well 2, vertical stratification does not seem to occur within the injection zone.

Except at regional monitor wells 2 and 3, the chloride concentration was approximately in the same ratio to the dissolved-solids concentration in most samples (about 0.60 at injection site 1, from 0.51 to 0.57 at injection site 2 and regional monitor well 1, about 0.40 at regional monitor well 2, and about 0.02 at regional monitor well 3).

Native Water Physical Properties

Pressure within the injection zone varies with structural elevation, and hence increases downdip, approximately south-southwest. The temperature of the native aquifer water was noted on geophysical logs from various wells (Hull and Martin, 1982). The average temperature gradient with depth is 0.0129°F/ft. Using this average, in the approximate 60-foot thickness of the most permeable part of the injection zone, the temperature would vary about 0.77°F.

A value of fluid density of 62.46 lb/ft^3 at 68°F, atmospheric pressure, and about 3,500 mg/L of dissolved solids, was measured for the native aquifer water in March 1977 from the north deep monitor well at injection site 2. Assuming linear coefficients for the variation of fluid density with temperature, pressure, and dissolved solids concentration (INTERCOMP Resource Development and Engineering, Inc., 1976), density could vary by about 0.2 lb/ft^3 from a pressure variation of about 1,000 lb/in^2 occurring as a result of aquifer dip, and could vary about 0.1 lb/ft^3 from a temperature variation of 10°F, about the areal variation observed. Pressure and temperature coefficients were based upon standard value (3×10^{-6} in^2/lb) for water compressibility and an average value ($0.0002°F^{-1}$) for the coefficient of thermal expansion (INTERCOMP Resource Development and Engineering, Inc., 1976). A rough estimate of the density dependence upon solute content, when the dissolved-solids concentration is less than 15,000 mg/L, is 0.05 lb/ft^3 per 1,000 mg/L of dissolved solids (American Public Health Association, 1976). A dissolved solids concentration variation of 9,000 mg/L, a lower estimate of the difference between the monitor wells at injection site 1 and the regional monitor well 2, would cause density to vary by about 0.45 lb/ft^3.

Thus, on a regional basis, the primary dependence of fluid density was upon the dissolved-solids concentration. On a local scale, the only appreciable density variations would occur at the injection sites as a result of the injection of wastewater with a density different from the native water and the local large increase of pressure. Temporary local variations would occur when injected fluid varies greatly in temperature from the native aquifer fluid.

Fluid viscosity varies with temperature and solute content (INTERCOMP, 1976). Since the aquifer temperature variation is slight and the viscosity difference between distilled water (0 mg/L dissolved solids) and seawater (31,500 mg/L dissolved solids) is slight, the viscosity of the aquifer fluid probably does not vary greatly throughout the study area. A value of 0.76 centipoise was measured (C. A. Pascale, oral commun., 1977).

Hydraulic Properties

Hydraulic conductivity is a parameter which provides a measure of the ability of a unit cross-sectional area of aquifer material to transmit fluid of a specific density and viscosity when subjected to a hydraulic gradient. If integrated vertically over the thickness of one or more geologic formations, possibly vertically heterogeneous, the result is the transmissivity parameter. In this study, the sparse set of direct field measurements were of transmissivity.

Transmissivity determinations from aquifer tests in secondary porosity layers can be unreliable because of inhomogeneous distributions of porosity and of channels for fluid flow. Nevertheless, the three similar values from injection site 1 (Faulkner and Pascale, 1975) are consistent with an estimate of 850 ft^2/d in that vicinity. The agreement of the larger two ranges of values from injection site 2 (C. A. Pascale, written commun., 1977) suggests an approximate transmissivity value of 1,500 ft^2/d in this area. Recovery and drawdown tests at the regional monitor well 1 (Pascale, 1976) established a range in transmissivity of 3,500-5,000 ft^2/d. At regional monitor well 2, a range of 230-520 ft^2/d was obtained. As single determinations at isolated locations within the secondary-porosity injection zone, these cannot be considered fully reliable estimates of the average transmissivity in their respective localities. In the vicinity of monitor well 2, the aquifer material consists of coarse clastics mixed with limestone, and the native aquifer water is less saline than at other localities. Solution of such material leads to a high degree of permeability, and the low salinity suggests strong flushing of the aquifer by recharge water from the north. Thus, the low value of transmissivity obtained at that location was considered doubtful.

Hydraulic conductivity tends to decrease significantly with increasing depth within the injection zone. As the north and south monitor wells at injection site 1 were drilled, measurements of the augmentation of flow from successive sections drilled were made (Foster and Goolsby, 1972). The measurements at the south monitor well began at the bottom of the casing 60 feet below the top of the lower limestone of the Floridan aquifer. Of the flow from the open hole below this level, 80 percent occurred in the first 40 feet, and the augmentation of flow gradually diminished to zero in another 124 feet. The measurements from the north monitor well began at the bottom of the casing, 55 feet below the top of the lower limestone. Of the flow from the open hole below this level, 66 percent occurred in the first 26 feet, and the flow from the remaining 156 feet was minimal. The data do not show whether the upper 55 to 60 feet of the injection zone contribute flow. Logging during the recent construction of injection well C is said to have shown "that the most porous zones are not in the upper part of the injection zone" (C. G. Hoffman, Monsanto Company, written commun., 1983).

At the primary and standby injection wells and north deep monitor well at injection site 2, flow meters were used to measure the velocity of flow at various depths while the wells were pumped or allowed to flow at constant rates (C. A. Pascale, written commun., 1977). At the primary injection well, the bottom of the casing is about 18 feet below the top of the lower limestone, and flow diminishes to zero in another 52 feet. At the standby injection well, the bottom of the casing is 25 feet below the top, and the flow diminishes to zero in another 60 feet. Only at the north deep monitor well do the data fail to indicate higher flow from the uppermost levels. However, this well was not fully developed when drilled, because of environmental considerations, and the flow meter data may not be representative.

The storage factor, in an artesian zone, is the measure of the aquifer's ability to absorb additional fluid mass of a particular density through the compression of the aquifer material and of the fluid itself. It is, thus, dependent upon the amount of existing pore space and the thickness of the layer (Lohman, 1972). If expressed as a quantity per unit aquifer thickness, the result is termed specific storage.

Few measurements of storage in the injection zone are available. Barraclough (1966) indicates a range of 0.001 to 0.0001 at injection site 1. More precise estimates are made by C. A. Pascale (written commun., 1977), who suggests values of 2.6×10^{-4} and 2.8×10^{-4} from an interpretation of data from tests at injection site 2 (Pascale, 1975). Since both latter values are from the same location within the study area, they do not show any areal variation of storage factor which might actually prevail.

Estimates of effective porosity ranging from 11 to 28 percent were obtained from the two injection sites and the two regional monitor wells (Faulkner and Pascale, 1975; Pascale, 1975, 1976). The latter value is best supported in that, together with data describing the vertical distribution of flow, it is consistent with the arrival time of injected waste at the standby injection well at injection site 2, assuming uniform isotropic flow from the primary injection well (Ehrlich and others, 1979).

Regional Flow System

The natural flow patterns within the injection zone are determined by its lithology, transmissive properties, and the location and type of boundaries, particularly those where recharge or discharge take place. These are the patterns which prevailed in the aquifer in its natural undisturbed state prior to the commencement of injection operations and which continue to influence the movement of injected waste.

Flow in coastal aquifers is often downdip towards subsea outcrops if no permeability barriers intervene. Given the nearly complete lack of water-level data from the injection zone prior to the construction of the injection systems, it was assumed that flow was downdip to the southwest, possibly discharging at a subcrop beneath the waters of the Gulf of Mexico. However, in subsequent years, geologic, hydraulic, and water-quality data were acquired which suggest a different interpretation.

Indications (J. A. Miller, written commun., 1978) of the displacement of the Ocala Limestone by faulting in an area to the northwest of the injection sites and of its thinning (or of the pinching out of the upper permeable part) to the west and southwest of the injection sites suggest a partial or complete barrier to flow in these directions. In addition, water-quality data from various injection and monitor wells suggest an interface of fresh and saline water, with freshwater to the northeast of the sites and stratified saline water increasing in concentration to the southwest.

The saline water could be unflushed depositional water. Or, if the faulting and thinning to the west and southwest does not constitute a total barrier to flow, the saline water could be seawater in limited hydraulic contact with the injection zone. However, the position of saline water many tens of miles inland from a possible injection zone subcrop to the southwest suggests that no freshwater discharge to the sea occurs there. If the presumed subcrop of the injection zone downdip to the southwest occurs at sufficient depth, the equivalent freshwater head would be so large as to retard freshwater discharge. It seems more likely that freshwater recharge from areas to the north where the injection zone is unconfined or poorly confined could either move toward the east or southeast or leak slowly upward throughout a large area. Because of the tightness of the Bucatunna confining layer, it is likely that recharge water moves southeast parallel to the saltwater interface towards either a southeastern undersea subcrop at higher elevation or towards some location where low water levels coincide with the pinchout of confining layers.

The best evidence of natural flow patterns are preinjection water levels. Exactly three such data are available. The preinjection water level at injection site 1 was 76 feet above sea level (Barraclough, 1966), measured as wellhead pressure by a transducer with a water-level readout (J. B. Martin, oral commun., 1984). A water level of 128 feet above sea level was recorded in 1961 at regional monitor well 3 near the Camp Henderson Lookout Tower on the Florida-Alabama border, and a value of 137 feet above sea level was the average of five water levels recorded at a well in Escambia County, Ala., from 1968 to 1970 (Marvin E. Davis, oral commun., 1977). Although the latter data were measured after the commencement of injection, the distance of the the well from injection site 1 and its proximity to the limit of the Bucatunna Clay, beyond which unconfined water levels were virtually unaffected by injection (because of the great difference in confined and unconfined storage factors), indicated that this water level probably changed little during 5 to 7 years of waste injection. The three cited data were adjusted to 84, 123 and 132 feet in reference to a common dissolved solids concentration of 5,000 mg/L.

Three control points were barely sufficient for interpretation, but others could be estimated from a knowledge of subsequently measured water levels known to be influenced by injection stress. Since the water-level response curves computed by the calibrated model matched the later data, they were assumed to be accurate estimates of the water-level change from the beginning of injection up till the time that measured water levels first became available. Such backward extrapolation at three widely spaced monitor wells provided estimates (adjusted to 5,000 mg/L of dissolved solids) of 77 feet at the deep test monitor well at injection site 2 and 46 and 86 feet, respectively, at regional monitor wells 1 and 2. The contouring is shown on figure 7.

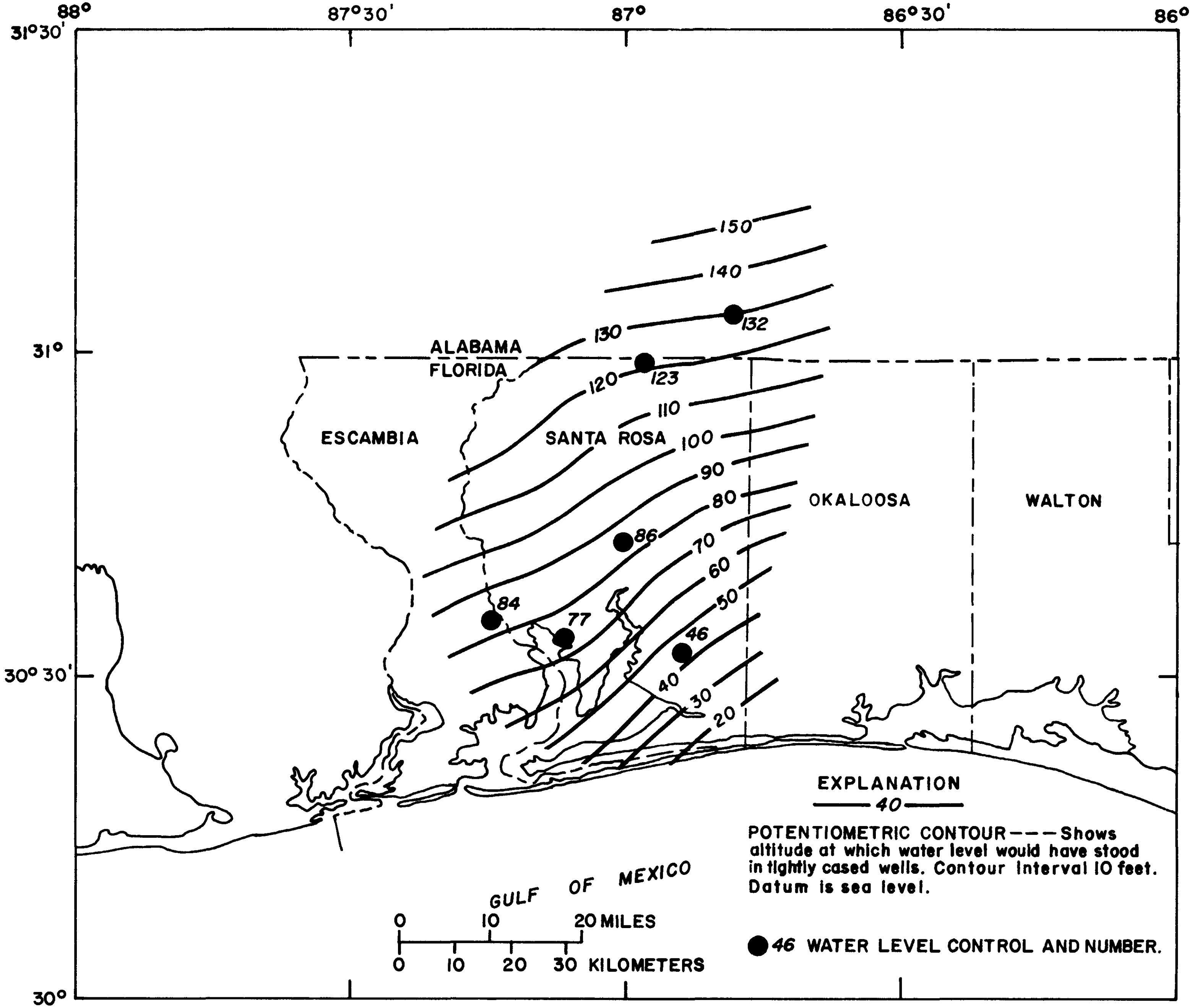

Figure 7.--Preinjection water levels in the injection zone inferred from known and reconstructed control points.

The data indicate a generally southeastward direction of flow in this region. A puzzling characteristic is the behavior of the contour lines in the space between the deep test monitor well (77 feet) and regional monitor well 1 (46 feet). If the first value were lower and the second higher, more uniform contour spacing would be the result. Marked variations in the transmissivity of the aquifer in this area may be indicated by the large water-level gradient between the two wells. The lack of an areal distribution of detailed geohydrologic information from the injection zone is highlighted by this feature and an examination of geophysical logs from test oil wells (J. A. Miller, oral commun., 1978) revealed no apparent anomalies.

A southeasterly flow regime was accepted as the conceptual model of the natural flow system in the injection zone. It was assumed that permeability barriers occurred to the northwest, west, and southwest of the injection sites, and that recharge water from the north flowed southeast toward areas of discharge. If the permeability barriers were only partially effective, the interpretation of the flow system would likely be unchanged. It was assumed that the Foshee, Pollard, and Jay Faults near the Florida-Alabama border were insufficient displacements to affect the integrity of the confining layer.

GENERIC DIGITAL SIMULATORS USED IN THE WASTE INJECTION STUDY

Finite-Difference Model for Aquifer Hydraulic Simulation in Two Dimensions

The mathematical basis of the U.S. Geological Survey two-dimensional flow model (Trescott and others, 1976) was described by Pinder and Bredehoeft (1968). Ignoring density-driven flow, Jacob (1950) used the law of conservation of fluid mass to obtain the second-order, linear, partial differential equation of flow in three dimensions:

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) = S_s\frac{\partial h}{\partial t} - A \qquad (1)$$

where $h=h(x,y,z,t)$ is hydraulic head (L)

K_{xx}, K_{yy}, and K_{zz} are components of hydraulic conductivity in three coordinate directions, where; $K_{ii} = \rho g k_{ii}/\mu$, $i = x,y,z$ (L/T)

ρ is density (M/L^3)

g is acceleration due to gravity (L/T^2)

μ is transient viscosity (M/LT)

k_{ii} is intrinsic permeability in the i^{th} coordinate direction (L^2).

$S_s = \phi\rho g(C_w + C_r)$ is specific storage (1/L)

where ϕ is porosity (dimensionless)

C_w is compressibility of water (LT^2/M)

C_r is elastic compressibility of the aquifer material (LT^2/M)

$A = A(x,y,z)$ is the sum of nonadvective sources and sinks of fluid, expressed as a rate per unit volume (1/T).

Equation 1 is reduced to an analogous equation in two dimensions that can be used to describe horizontal planar flow when vertical flow is negligible. The reduction is done by vertical integration of equation 1 and results in the following second-order, linear, partial differential equation upon which the model is based:

$$\frac{\partial}{\partial x}\left(T_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_{yy}\frac{\partial h}{\partial y}\right) + \left(K_z\frac{\partial h}{\partial z}\right)_{z_2} - \left(K_z\frac{\partial h}{\partial z}\right)_{z_1} = S\frac{\partial h}{\partial t} - V \qquad (2)$$

where $T_{xx} = bK_{xx}$, $T_{yy} = bK_{yy}$ are transmissivities (L^2/T)

$S = bS_s$ is storage coefficient (dimensionless)

$b = b(x,y)$ is thickness of aquifer layer (L)

$V = V(x,y)$ is the sum of sources and sinks of fluid per unit area (L/T).

K_{xx}, K_{yy}, and S_s are considered to be vertically averaged parameters, and hydraulic head is also treated as a vertically averaged quantity. The third and fourth terms on the left hand side of equation 2 represent vertical flow (leakage) through the top and bottom surfaces, respectively.

Equation 2 is solved by using the finite-difference approximation method (Trescott and others, 1976) in which the planar area modeled is represented by a geometric grid and an equation is written for a nodal point within each grid cell. The version of the model applied in this study incorporates a variable block-centered grid. The approximation of the second-order spatial derivatives is written entirely at the new time level (fully implicit), and the approximation of the first-order time derivative is a backward difference. The method leads to system of linear equations, and three methods of matrix decomposition are available in the model for solving the system. In this study, the strongly implicit procedure (SIP) was used.

The computer model represents areal heterogeneities in transmissivity by distributing parameter values among the grid nodes. Transmissivity may be homogeneously anisotropic throughout the area modeled, and assigned values are assumed to represent local fluid density and viscosity and permeability of the aquifer material. Storage parameter values may be similarly distributed, and reflect the local fluid density, porosity of the aquifer material, and aquifer thickness. Spatial variations in density are assumed to be small, however, as flow driven by density gradients is not simulated by the model.

The model requires the specification of a no-flow boundary (zero transmissivity) around the periphery of the area modeled. Adjacent grid blocks may be constrained to have time-invariant values of hydraulic head. Water flux across these boundaries in simulation time steps is a function of the difference in head between the constant head node value and the head computed for the adjacent block, and of the local transmissivity. Time-invariant flux boundary conditions can also be specified. Initial conditions in the aquifer must be directly specified for transient simulations. In this study, all boundaries were treated as zero-flow (impermeable) or constant-head situations. Since the aquifer layer modeled was located between two tight confining layers, model components for simulating vertical leakage were not used.

The source term in equation 2 is for the general purpose of representing pumping or injection through wells and recharge or discharge by various means such as evapotranspiration. Its application in this study was to represent the two injection wells.

The computer program permits user control of time-step length. The user may compute a steady-state simulation directly in one time step by specifying storage coefficient to be zero in all grid blocks for which head values are computed. This has the effect of deleting the time derivative from the model equation, which thereby becomes an equation for steady-state conditions.

Finite-Difference Model for Simulation of Aquifer Pressure Distribution and Solute and Thermal Transport in Three Dimensions (SWIP)

The SWIP (subsurface waste injection program) model was developed under sponsorship of the U.S. Geological Survey by INTERCOMP Resource Development and Engineering, Inc. The model was designed to simulate hydraulic effects and solute and thermal transport in deep, confined aquifers used for liquid waste disposal. Recent modifications permit application to a wider variety of physical prototypes. The solution techniques, verification testing, and various computer aspects have been the subject of a U.S. Geological Survey report (INTERCOMP, 1976). A revised version was documented later (INTERA Environmental Consultants, Inc., 1979).

The nonlinear partial differential equation solved for the pressure field in three-dimensional Cartesian coordinates (X, Y, and Z) and time (t) is:

$$\frac{\partial}{\partial x}\left(\frac{\rho k_x}{\mu}\frac{\partial p}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\rho k_y}{\mu}\frac{\partial p}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{\rho k_z}{\mu}\left[\frac{\partial p}{\partial z} - \rho g\right]\right) = \rho\phi_o C_r\frac{\partial p}{\partial t} \tag{3}$$

$$+ \phi\left[\rho_o C_w\frac{\partial p}{\partial t} + \rho_o C_T\frac{\partial T}{\partial t} + \frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t}\right] + q'$$

Where the three dependent variables are:

$p = p(x,y,z,t)$ is pressure (M/LT^2)

$T = T(x,y,z,t)$ is temperature (temperature units),

$C = C(x,y,z,t)$ concentration expressed as a unitless fraction, where $C \varepsilon \langle 0,1 \rangle = \langle C_o,C_1 \rangle$,

and where:

$\rho = \rho(p,T,C)$ is density (M/L^3)

$\mu = \mu(T,C)$ is transient viscosity (M/LT)

k_x, k_y, and k_z are permeabilities in the three coordinate directions (L^2)

g is gravitational acceleration (L/T^2)

C_r is compressibility of the aquifer material (LT^2/M),

C_w is compressibility of water (LT^2/M),

C_T is coefficient of thermal expansion (reciprocal temperature units),

$\phi = \phi_o(1+C_r[p-p_o])$ where ϕ_o is porosity (dimensionless) at some reference pressure p_o

ρ_o is density at reference conditions p_o, T_o, and C_o

$\frac{\partial \rho}{\partial C}$ is estimated as $\rho(p_1,T_1, 1_1) -\rho(p_1,T_1, 0_o)$ where p_1 and T_1 are some arbitrary reference conditions,

q' is the sum of nonadvective sources and sinks of fluid, expressed as mass flux per unit volume (M/L^3T).

All of the terms on the right-hand side except q' constitute the change in storage term. The properties of the fluid in the aquifer are considered to vary with temporal variations in temperature, concentration of solute, and pressure. The functional dependence of fluid density and viscosity upon temperature and solute fraction is incorporated into the model computations. The hydraulic conductivity values in the advective terms are also corrected whenever fluid properties change. The terms on the left-hand side of the equation are a representation of flow that takes into account spatial gradients in density.

The nonlinear partial differential equation for the transport of solute in three dimensions (INTERCOMP, 1976) is as follows. An analogous equation is also derived by Konikow and Grove (1977).

$$\frac{\partial}{\partial x_i}\left(\frac{C\rho k_{ii}}{\mu}\frac{\partial p}{\partial x_i}\right) + \frac{\partial}{\partial x_i}\left(\rho E_{ij}\frac{\partial C}{\partial x_j}\right) = C\rho\phi_o C_r\frac{\partial p}{\partial t} + \phi C\left[\rho_o C_w\frac{\partial p}{\partial t} + \rho_o C_T\frac{\partial T}{\partial t} + \frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t}\right] + \rho\phi\frac{\partial C}{\partial t} + Cq + \Sigma\, C_i q_i \tag{4}$$

where the summation convention is used, and $x_1 = x$, $x_2 = y$, and $x_3 = z$ are the three Cartesian coordinates.

E_{ij} are components of the dispersion tensor (L^2/T) and

$E_{ij} = E_{ij}(u,\alpha_L,\alpha_T,D_M)$ where u is fluid velocity

α_L,α_T are longitudinal and transverse dispersivities

D_M is molecular diffusion

and other terms are as for equation (3).

Dispersion results in the presence of mixed injected and native waters on either side of the boundary which would delimit the injected water by virtue of its simple geometric bulk displacement of the native water. The dispersion terms are the macroscopic representation of a set of small-scale phenomena including nonuniformities in fluid properties and aquifer properties, nonuniformities in fluid velocity, and molecular diffusion. Except for the molecular diffusion component, the magnitude of the dispersion coefficients are represented as having a linear parametric dependence upon the velocity of flow. This dependence is represented by two independent dispersivity parameters, related to dispersion in and perpendicular to the direction of flow (Scheidegger, 1961).

The model equations for pressure, concentration, and temperature are solved with finite difference techniques in which the aquifer is represented in Cartesian coordinates (X, Y, Z) as a one-, two-, or three-dimensional, variable, block-centered grid, or in cylindrical coordinates (r, z) as a one- or two-dimensional grid. Several differencing schemes are provided as options for solving the concentration and temperature equations. The user may specify that the spatial derivative terms in the concentration and temperature equations be evaluated at the new time iteration level (implicit) or centered in time between old and new iterate levels (Crank-Nicholson). In addition, the advective terms may be differenced by a backward or a centered scheme.

The resultant system of linear equations can be solved either by a direct method (ADGAUSS) due to Price and Coats (1973), which relies upon ordering methods to reduce computing time and storage requirements from those required by earlier direct methods, or by an iterative method (L2SOR). Because the decomposition by L2SOR of the large matrices used in the study required less storage than the direct method, L2SOR was used.

SWIP provides for the spatial variation of some parameters describing aquifer characteristics by a nodewise assignment of values, while other parameters are considered to describe areally homogeneous properties. Intrinsic permeability in each coordinate direction is input by nodal distributions of hydraulic conductivity values at specified conditions of pressure, temperature, and solute fraction. Aquifer storativity (Lohman, 1972) is specified by inputs of porosity, layer thickness, fluid density, and compressibilities of water and of the aquifer material. Porosity and layer thickness may be spatially distributed. Coefficients are entered to describe the thermal behavior of the fluid and aquifer.

Fractional values are entered to describe the concentration of some actual or hypothetical solute in the aquifer resident fluid and in any fluid influxes. The extreme values of concentration fraction (0.0 and 1.0) are assigned density values at some reference temperature and pressure conditions, and this density contrast is incorporated into all computations.

SWIP provides for such hydraulic boundary flux specifications as no-flow, constant flux, or flux controlled by constant pressure. Where a boundary flux condition is not specified, SWIP assumes zero flux. Where constant boundary pressures are specified, constant values of temperature and concentration fraction are also specified. Various time-varying boundary conditions may also be specified, but in this study zero flux and constant boundary conditions were all that were needed. Initial conditions for pressure, concentration fraction, and temperature throughout the modeled area are also specified.

The computer code was modified to convert pressure values to hydraulic head values upon output for convenience in making comparisons with field data. The value of density used for the conversion at each node point was computed by the linear formula of INTERCOMP (1976), using nodal values of temperature and concentration and using the average of the nodal value of pressure and atmospheric pressure. These values were considered to most accurately represent the average condition of the water in the water column.

APPLICATION OF MODELS TO SIMULATE HYDRAULIC EFFECTS OF WASTE INJECTION

Model Calibration

Mathematical models of aquifer systems often include parametric representations of physical processes, in which the values of parameters are used to specify the quantitative level of each process. Simulation consists of selecting the correct values of these parameters, which may be determined by direct or indirect measurements from the aquifer. If all such parameter values are known, and the model design is correct, the model is an exact representation, except for mathematical approximation error, of the response of the aquifer in terms of some measured variable (hydraulic head) to any level of imposed stress (injection or withdrawal), and can be used with confidence for prediction.

Usually, however, some parameters are unknown or poorly known. If enough parameters are well-known, the remaining ones can be determined by making a series of computations with a range of values of the unknown parameters in which dependent variables computed by the model in response to a simulated stress are compared with actual measurements of these variables when this level of stress occurs in the aquifer. This process is called calibration.

A steady-state simulation solves for the equilibrium response to a set of conditions, while a transient simulation solves for the response as a function of time starting with a nonequilibrium combination of initial conditions and imposed stresses. In the steady-state simulation of a fully confined aquifer with the two-dimensional flow model, the dependent variable is hydraulic head, and required parameters are transmissivity, location and type of boundaries, and boundary head or flux values. In transient hydraulic simulations with this model, the dependent variable is the change in hydraulic head and the required parameters are transmissivity, storage coefficient, and location and type of boundaries. The magnitude and rate of water-level change may sometimes be used independently as points of comparison. Steady-state (equilibrium) initial conditions are used in transient simulations so that the hydraulic response to a newly imposed stress can be isolated from the hydraulic response to an unsteady combination of initial and boundary conditions. Values describing constant head or flux levels at boundaries are not parameters affecting hydraulic response in transient simulations if such steady initial conditions are used, by virtue of the linearity of the partial differential equation describing two-dimensional flow.

Often, a sensitivity analysis, in which some parameter is varied while others are held constant, is made to determine which parameters are of greatest importance in causing variation of the dependent variable.

Approach

As the nearest distance between an injection and observation well was over 1,000 feet, observed hydraulic data were assumed to represent the condition of lateral flow. Because upward leakage through confining layers was considered negligible and layers below the injection zone were much lower in hydraulic conductivity, it was appropriate to simulate hydraulic effects with a single-layer areal model of lateral flow tightly confined above and below. The hydraulic boundaries of the aquifer include pinch-outs, lithologic facies changes, vertical faulting, and saltwater interfaces. Either zero-flux or constant-head conditions characterized all boundaries. The two-dimensional flow model was appropriate for simulation of these flow and boundary conditions. The use of this model for hydraulic simulation was considered advantageous in comparison to SWIP because of lower computer costs, even though the SWIP hydraulic solution, taking into account minor density effects, was slightly more accurate. The aquifer was assumed to be isotropic with respect to hydraulic properties within the plane of flow.

Hypotheses concerning the natural, prestress regional flow in the aquifer were tested with steady-state simulations. Precise simulation would have required sufficient data to accurately describe preinjection water levels throughout the study area. Such a simulation would also benefit from a good areal distribution of transmissivity measurements and an unambiguous description of hydrologic conditions in all areas where boundaries to the flow system were presumed to occur. As available data were limited, the accuracy achievable was also limited, and a highly generalized model was considered a reasonable objective. This result would lend some credence to the identification of boundaries, but would not constitute a precise validation of the choice of transmissivity values or their spatial distribution.

Transient simulations attempted to match water-level responses observed at monitor wells following changes in average injection rate, in order to lend more credence to choices of transmissivity and storage coefficients and the location and types of boundaries. Because of the lack of preinjection water-level data and the generalized nature of the prestress steady-state simulation, absolute water levels could not be used as a basis for comparison. Considerable water-level response data from a few scattered locations were available for the transient calibration. However, the sparse areal distribution of the data and poor definition of some aquifer boundaries ruled out precise areal transmissivity or storage maps as an objective of the analysis, even given good water-level change matches at several observation points. Superposition of the transient and steady-state solutions, by using the latter as initial conditions for the transient runs, provided convenient but highly generalized portrayals of the approximate regional water-level distribution at various times after injection began.

The first transient simulation with the two-dimensional flow model assumed that the aquifer was practically infinite in all directions. Within the very large area of the model, it was assumed that there were no natural hydraulic boundaries such as barriers to flow or locations where the quantity of recharge or discharge was governed by time-invariant water levels. This simulation represented the case in which flow system boundaries were so distant from the injection stress that water-level increases at the boundaries would be negligible. These simulations were considered a not unrealistic approximation of the injection zone, as natural flow system boundaries were located relatively far from the two injection systems. In subsequent transient simulations, the hydraulic influence of each known or presumed flow system boundary was assessed with an image-well technique. This was followed by the construction of a model in which all such natural boundaries were represented, which was used for both steady-state and transient simulations. The final hydraulic model consisted of replicating these simulations with the more sophisticated SWIP simulator.

Adaptation of Data Base for Modeling

Hydraulic characteristics of the aquifer were estimated for model calibration on the basis of the data acquired during construction of the injection systems and monitor wells. Monthly average injection rates were discretized into long-term averages for a series of consecutive pumping periods (figs. 3 and 4). The choice of time intervals for the discretization was based upon the variability in the actual pumping rates and the precision desired in comparing observed and computed values. Since most comparison water-level data were measured after 1971, injection rate data after that year were discretized into shorter time intervals. From the commencement of injection at site 2 in June 1975 until 1978, injection rates remained at nearly the same level at both sites, so a single average at each site (2,300 gal/min at site 1 and 550 gal/min at site 2) was used for simulation time periods beginning with June 1975. Injection rate data for 1978 were the latest available during the active phase of this investigation.

Water-level data, expressed with respect to land-surface datum were quite sparse in areal distribution, but accurate for long time periods where they were available. These data were almost nonexistent prior to 1970, when the south and north monitor wells were drilled near injection site 1. Earlier pressure data were obtained from the deep monitor well beginning in 1963. Collected twice a month, but sensitive to hourly fluctuations in injection pressure, the data displayed a trend that was largely obscured by the short-term rate fluctuations. Beginning in 1968, the data were affected by chemical reactions dissolving the aquifer material about the well. This caused a drop in pressure relative to the injection rate. These pressure data were not considered useful for model calibration of acceptable precision.

The distribution of water-level control points in the proximity of the injection systems included the north and south monitor wells near injection site 1 and the deep test monitor well, standby injection well, and north monitor well near injection site 2. Distant control points were the three regional monitor wells.

Density effects at the deep test monitor well, from allowing the well to flow during the winter of 1972-73 (saltier water) and from perforating the well in October 1973 (fresher water), are evident from its water-level hydrograph (Pascale and Martin, 1977, p. 15), which clearly shows discontinuities in the water-level curve at those times. This demonstrated the need to make water-level data adjustments reflecting changes in the dissolved solids concentration of water in the various monitor wells. The formula used for this adjustment was:

$$\Delta h = \frac{pC}{\rho_o} \left(\frac{1}{G_o} - \frac{1}{G_t}\right) \tag{5}$$

where Δh is the water-level correction

p = the local pressure

C = 144 in^2/ft^2, a conversion factor

ρ_o = 62.4 lb/ft^3, the weight density of water without dissolved solids

G_o = a selected standard value of specific gravity

G_t = specific gravity of water column at time t.

Using this formula, corrections as large as 5 feet were computed for various time sequences of water-level observations from monitor wells at the two injection sites. Corrections as large as 10 feet were also applied on a regional basis, as the dissolved solids concentration at water-level control points varied from near zero (regional monitor well 3) to 10,000-13,500 mg/L (injection site 1) and wellhead pressure and water-level measurements reflected the local aquifer water density. The corrections were based upon the apparent salinity of the water columns in the wells at various times, and this salinity may have differed slightly from the regional average salinity in the injection zone.

An arbitrarily selected common salinity standard of 5,000 mg/L dissolved solids, less than the 10,000-13,500 mg/L characteristic of injection site 1 and the 7,500 mg/L characteristic of injection site 2, was used as a standard, or common, value. This meant, in strict mathematical terms, that transmissivity and storage parameters determined by model calibration were valid for the water density corresponding to 5,000 mg/L dissolved solids and should be adjusted to the local native water density for comparison with field determinations of hydraulic characteristics. This would be done by multiplying by the ratio of the densities or alternatively, by the ratio of the specific gravities. However, actual corrections were so small as to be well within measurement error. For instance, the calibrated model transmissivity of 850 ft^2/d for injection site 1 would convert to about 855 ft^2/d, and the value of 1,500 mg/L for injection site 2 would convert to 1,503 ft^2/d.

Based upon regional salinity estimates of 12,200 mg/L of dissolved solids (site 1) and 7,500 mg/L of dissolved solids (site 2), rather than water-column values, height corrections for 1978 water columns of about 1,750 feet at the south monitor well (injection site 1) and about 1,700 feet at the deep test monitor well (injection site 2) were about 9.5 feet and 3.2 feet. The corresponding water-level changes during the time periods of data collection (about 55 and 80 feet, respectively) would only vary by 0.3 feet and 0.15 feet, respectively. The water-level change (about 230 feet) at the south monitor well (injection site 1), where initial water levels were known within a few feet, would be corrected only by about 1.25 feet. This shows that the regional density corrections were unimportant for the simulation of water-level changes, but could have been of some importance for attempts to simulate the regional flow system, though their significance was reduced by the scanty data base of only three measured pre-injection water levels. In view of this, the use of the salinity correction to refine the regional flow system simulation was probably an unwarranted search for additional precision. Assuming the hydraulic parameters to contain the dependence on density, although requiring a uniformity assumption to be applied to large sections of the aquifer, would have been an approximation of adequate precision for this study.

Simulation of Effectively Unbounded Aquifer Using Two-Dimensional Flow Model

Model Design and Calibration Techniques

The 1,025 feet between the primary injection well and the deep test monitor well at injection site 2 was the shortest distance between an injection well and a monitor well open to the injection zone. Inaccurate model computations of water-level values at the deep test monitor well in early simulations revealed the need to interpose several grid blocks between the wells in both coordinate directions. This demonstrated the need for fine grid definition in the area about each of the two injection sites located 8 miles apart. It was possible to considerably reduce the number of grid nodes by making the two injection sites colinear in the grid. This was done by orienting the positive Y-axis about 10 degrees clockwise from north. Since the two site 1 injection wells were merely 1,300 feet apart, their combined effect on water levels at the north and south monitor wells, the nearest observation wells, would be indistinguishable from that of a single injection well, so they were simulated as one well at the location of injection well A (fig. 1).

A factor of 2.0 was chosen as the maximum dimension expansion between adjacent grid blocks. The use of much larger expansion factors early in the study led to incorrect model computations. Model runs were made using the final grid design (table 1) and incorporating an assumption of areally uniform hydraulic parameters (transmissivity and storage coefficients). Computed water-level changes at various observation well sites were compared with the values predicted by the Theis equation, which is also based upon uniformity assumptions. Results showed agreement within 1.0 foot at locations where over 200 feet of water-level buildup occurred, and verified that the grid scheme was not introducing appreciable error.

Table 1--Spatial discretizations of the various hydraulic models

[Vertical and horizontal grid cell lengths in feet]

[MONS--Injection wells, site 1; SDMW--South monitor well, injection site 1; NDMW--North monitor well, injection site 2; AMCY--Primary injection well, injection site 2; DTMW--Deep test monitor well, injection site 2; SBIW--Standby injection well, injection site 2; DMWN--North Monitor well, injection site 2; RMW1--Regional monitor well 1; RMW2--Regional monitor well 2; RMW3--Regional monitor well 3]

Y-AXIS

Two-dimensional flow model: Unbounded aquifer Index	Unbounded aquifer Size	Natural boundaries Index	Natural boundaries Size	SWIP Index	SWIP Size	SWIP Well
1	25,000	1	75,000	--	------	----
2	50,000	2	75,000	--	------	----
3	100,000	3	50,000	1	50,000	----
4	141,825	4	50,000	2	50,000	----
5	141,825	5	50,000	3	50,000	----
6	100,000	6	50,000	4	50,000	----
7	53,229	7	53,229	5	53,229	----
8	24,000	8	24,000	6	24,000	----
9	12,000	9	12,000	7	12,000	----
10	6,000	10	6,000	8	6,000	----
11	3,000	11	3,000	9	3,000	----
12	1,500	12	1,500	10	1,500	SDMW
13	2,259	13	2,259	11	2,479	----
14	1,522	14	1,522	12	1,400	----
15	808	15	808	13	745	SBIW
16	546	16	546	14	546	DTMW
17	400	17	400	15	365	----
18	200	18	200	16	200	----
19	100	19	100	17	100	AMCY MONS
20	200	20	200	18	200	----
21	400	21	400	19	400	----
22	800	22	800	20	800	----
23	505	23	505	21	505	----
24	1,000	24	1,000	22	1,000	RMW1
25	1,652	25	1,652	23	1,652	----
26	1,738	26	1,738	24	1,738	----
27	1,182	27	1,182	25	1,182	DMWN
28	1,184	28	1,184	26	1,184	NDMW
29	2,200	29	2,200	27	2,200	----
30	4,400	30	4,400	28	4,400	----
31	8,421	31	8,421	29	8,421	----
32	8,800	32	8,800	30	8,800	----
33	12,600	33	12,600	31	12,600	----
34	10,000	34	10,000	32	10,000	----
35	5,000	35	5,000	33	5,000	RMW2
36	10,000	36	10,000	34	10,000	----
37	15,554	37	15,554	35	15,554	----
38	20,000	38	20,000	36	20,000	----
39	40,000	39	40,000	37	40,000	----
40	40,000	40	40,000	38	40,000	RMW3
41	40,000	41	40,000	39	40,000	----
42	80,000	42	80,000	--	------	----
43	80,000	43	80,000	--	------	----
44	103,650	--	------	--	------	----
45	100,000	--	------	--	------	----
46	50,000	--	------	--	------	----
47	25,000	--	------	--	------	----

X-AXIS

Two-dimensional flow model: Unbounded aquifer Index	Unbounded aquifer Size	Natural boundaries Index	Natural boundaries Size	SWIP Index	SWIP Size	SWIP Well
1	25,000	--	-------	--	------	----
2	50,000	--	-------	--	------	----
3	52,800	--	-------	--	------	----
4	100,000	1	100,000	--	------	----
5	161,172	2	50,000	1	50,000	----
6	128,000	3	50,000	2	50,000	----
7	64,000	4	64,000	3	64,000	----
8	32,015	5	32,015	4	32,015	----
9	24,000	6	24,000	5	24,000	----
10	12,000	7	12,000	6	12,000	----
11	6,000	8	6,000	7	6,000	----
12	3,000	9	3,000	8	3,000	----
13	1,500	10	1,500	9	1,500	NDMW
14	2,282	11	2,282	10	2,282	----
15	1,600	12	1,600	11	1,600	----
16	800	13	800	12	800	----
17	400	14	400	13	400	----
18	200	15	200	14	200	----
19	100	16	100	15	100	MONS
20	200	17	200	16	200	----
21	400	18	400	17	400	----
22	800	19	800	18	800	----
23	1,000	20	1,000	19	1,000	----
24	961	21	961	20	961	----
25	1,500	22	1,500	21	1,500	SDMW
26	3,000	23	3,000	22	3,000	----
27	6,000	24	6,000	23	6,000	----
28	9,000	26	9,000	24	9,000	----
29	7,903	26	7,903	26	7,903	----
30	6,400	27	6,400	26	6,400	----
31	3,200	28	3,200	27	3,200	----
32	1,600	29	1,600	28	1,600	----
33	800	30	800	29	800	----
34	400	31	400	30	428	----
35	200	32	200	31	220	DTMW
36	208	33	208	32	160	----
37	192	34	192	33	192	----
38	100	35	100	34	100	AMCY
39	135	36	135	35	135	----
40	200	37	200	36	200	SBIW
41	400	38	400	37	400	----
42	800	39	800	38	800	----
43	899	40	899	39	1,554	----
44	1,500	41	1,500	40	2,410	DMWN
45	3,000	42	3,000	41	2,545	----
46	4,874	43	4,874	42	4,317	----
47	8,854	44	8,853	43	8,300	RMW3
48	5,000	45	5,000	44	5,000	RMW2
49	10,000	46	10,000	45	10,000	----
50	18,510	47	18,510	46	18,510	----
51	10,000	48	10,000	47	10,000	----
52	5,000	49	5,000	48	5,000	RMW1
53	10,000	50	10,000	49	10,000	----
54	20,000	51	20,000	50	20,000	----
55	40,000	52	40,000	51	40,000	----
56	80,000	53	80,000	52	60,000	----
57	160,000	54	80,000	53	60,000	----
58	100,000	55	80,000	--	------	----
59	65,596	--	-------	--	------	----
60	50,000	--	-------	--	------	----
61	25,000	--	-------	--	------	----

A very large area (251.6 miles square) was included within the grid design for the effectively unbounded aquifer simulation so that appreciable hydraulic effects of injection would not reach the simulation boundaries even after 15 years of waste injection at injection site 1. This permitted the specification of constant head conditions at those boundaries. The two injection wells, about 8 miles apart, were located near the center of the grid, so that each injection well was at least 120 miles from the nearest point on a boundary. Grid block size varied from cells 100 feet square containing the injection wells to cells 160,000 feet square near the northeastern boundary (table 1).

Only limited evidence was available for a regional distribution of transmissivity values, and that indicated an increase from injection site 1 toward regional monitor well 1 in the east-southeast direction (along the X-axis of the grid). The only distribution of values considered to have some basis in measured data was the assignment of uniform values to vertical strips in the grid, corresponding to strips of geographical area oriented about 10° clockwise from north. These strips extended from the lower boundary to the upper boundary of the grid. The one farthest to the left extended to the left boundary of the grid, and the one to the right extended to the right boundary. Initial values assigned to the strips were based upon aquifer tests at the two injection sites and at regional monitor well 1. The transmissivity estimate at regional monitor well 2 was ignored, as it did not appear to correlate with lithology and water quality. The number of strips, their assigned uniform values, and the position of the boundaries between them were adjusted during calibration of the transient response to injection, and received additional testing in subsequent simulations. Ultimately, values of 850, 1,500, and 4,000 ft^2/d were selected for three strips. The two vertical lines of demarcation were approximately midway between the two injection sites and about 6-$^2/_3$ miles east-southeast of injection site 2.

Since the two relatively precise field determinations of storage coefficient were from only one location in the study area, there was no basis for an areal distribution of values. Model calibration was done using a single value for the entire region, and the values tested in model runs were similar to the two measured ones. Ultimately, a value of 2.75×10^{-4} was selected.

In simulation runs, the amplitude and slope of the rising or falling computed water-level response to increases or decreases of average injection rate were studied. Cumulative positive and negative biases were considered indicative of parameter error. It was observed that certain types of amplitude or slope deviations were characteristic of transmissivity or storage coefficient errors in a part of the model grid distant from the water-level observation point, and other types of deviations characteristic of parameter errors in the neighborhood of the observation point. Parameter errors affecting both local and distant areas of the model grid could lead to a combination of types of amplitude and slope deviations.

The explanation of these different effects of parameter error is complex, relating to the greater or lesser water-level gradients required to transmit water in the local or distant area when the aquifer is more or less transmissive or has greater or lesser storage capacity. The two basic curve deviations are (1) cumulative bias in water levels at the observation point (caused, for example, by distant area transmissivity errors), and (2) response curve amplitude errors, in which the initial water-level change was too large or too small, but the slope of the subsequent water-level response curve is approximately correct (local area transmissivity or storage coefficient errors). These effects were the subject of sensitivity analyses to be described in a subsequent section.

Simulation of Water-Level Changes

The calibration of the effectively unbounded aquifer simulation produced a satisfactory match between computed and observed water-level responses to injection at monitor wells near the two injection sites. At the more distant regional monitor wells 1 and 2, the slopes of computed response curves were somewhat different from those of the observed curves. At the still more distant regional monitor well 3, model computations portrayed a water-level rise of 18 feet by October 1978, but observed water levels actually declined 13 feet by October 1977. These distant well discrepancies could have resulted from disregarding the effect of actual aquifer boundaries rather than being the result of imprecise model calibration. The decline at regional monitor well 3 also may have been caused by local pumping for water supply or by large-scale pumping from the upper limestone in Okaloosa County. Rather than refining this calibration, an assessment of the boundary effects and their incorporation into the model seemed to be the best direction for further efforts.

Assessment of Boundary Effects

Aquifers are said to be delimited by flow system boundaries where flow is barred (impermeable boundaries) or where flow is controlled by time-invariant water levels or fluxes (constant head or flux boundaries). Based upon estimates of the northern and eastern extent of the Bucatunna Clay member (fig. 6), the nearest point of its absence to the injection wells is where it pinches out about 37 miles northeast of injection site 1 and about 32 miles northeast of injection site 2. The fault to the west of the study area is approximately 50 miles from site 1 at its nearest point. The perpendicular distance from site 1 to the model boundary to the southwest representing the apparent pinchout of the upper, more transmissive part of the injection zone is also about 50 miles. The nearest point of the presumed Gulf of Mexico outcrop to the south of the injection sites is estimated to be from 75 to 100 miles.

Three sensitivity analyses were performed to test whether water levels computed by the partially calibrated effectively unbounded aquifer simulation would change appreciably when the hydraulic influence of the northeastern, western, and southwestern features were represented in the model by image wells. Regarded as boundaries to the flow system, the influence of each feature was assessed independently. The Gulf of Mexico outcrop was assumed to be too distant to have an appreciable effect upon water-level changes at control points.

In image-well analyses (Lohman, 1979), a boundary is considered to be a straight line, and an image well is located an equal distance on the opposite side of the boundary along an extension of the perpendicular from the real well to the boundary. Where an aquifer becomes unconfined at the pinchout of a confining layer, long-term average water levels might remain approximately constant even while they change in the confined section under the influence of imposed stresses, because factors of unconfined storage are usually several orders of magnitude larger than confined storage factors. Thus, assuming time-invariant water levels where the aquifer is not confined, the image of an injection well should have a withdrawal rate equal to the rate of the injection well, so that water levels along the straight-line boundary representing the confining layer pinchout are maintained constant by equidistant pumping and injection at rates equal in absolute magnitude.

Following this procedure, image wells corresponding to the Monsanto Company and American Cyanamid Company injection wells were located on the far side of the straight line approximation of the northeast Bucatunna pinchout. Conveniently, the two images nearly coincided with the center of the same grid cell, so a single image well was located at that node with a pumping rate equal to the combined rates of the injection wells.

Differences from the effectively unbounded aquifer simulation water-level changes were appreciable at regional monitor well 3, in close proximity to the approximate boundary. The previous 18-foot rise was reduced to a 2-foot rise during the same time period (July 1963 to October 1978). At regional monitor well 1, the 12.6-foot rise from April 1974 until October 1978 was reduced to 10 feet. At regional monitor well 2 to the north, the 14.3-foot rise was reduced to 11 feet. The slopes of the revised response curves matched those of the observed water levels, suggesting that a model incorporating the northeast boundary and the previously selected hydraulic coefficients would nearly match water-level changes at most regional control points. Near injection site 2, the image well pumping caused computed water-level changes from June 1975 to October 1978 to be 1.5-2.0 feet less than previously computed. At injection site 1, there was about 4.0 feet less of a water-level change in the 15-year injection time period from 1963.

An impermeable boundary is represented as a flow divide (Lohman, 1979) by making the injection well image another injection well with the same rate. This was done for impermeable boundaries to the west and southwest of the injection sites. The observation well locations nearest to both boundaries were the north and south monitor wells at injection site 1 where the change in computed water levels was less than 0.2 foot and within the closure criterion for the model computations. Thus, the hydraulic influence of these boundaries upon water-level changes at control points used to calibrate the model was negligible during the time period of the simulation.

If water-level control points had been located closer to the impermeable boundaries, the corresponding response curves could have shown considerable variation in the tests. If the simulation time period had been appreciably longer, the influence of the impermeable boundaries at existing control points would have been greater, as the aquifer had not yet reached hydraulic equilibrium with the injection stress.

Incorporation of Natural Aquifer Boundaries Using Two-Dimensional Flow Model

Boundary Representation

Impermeable boundaries were specified in the model as zero-flux. The interface with the Gulf of Mexico to the south represented the likelihood of some form of discharge under the control of average sea level head. A convenient representation was as a constant head boundary. Northern, northeastern, and eastern model boundaries corresponding to the cropping out (to the north) and pinching out (to the northeast and east) of the confining layer, where long-term average water levels were assumed to be approximately constant, were represented as constant head.

Actually, unconfined water levels to the northeast and also to the east (where the Bucatunna Clay pinches out approximately 20 miles east of Fort Walton Beach in southern Okaloosa County) declined during the 15-year time span of injection until 1978. A water-level decline of 13 feet was observed at regional monitor well 3, about 8 miles within the area of confinement, and a water-level decline of about 6 feet was measured to the northeast at the Alabama observation well, about 2 miles outside the area of confinement. In the vicinity of the pinchout east of Fort Walton Beach, a water-level decline of 30 to 40 feet was observed.

The decline east of Fort Walton Beach, and also possibly the decline northeast of the injection sites are widely believed to be the result of heavy pumping from the confined upper limestone of the Floridan aquifer in the Fort Walton Beach area. That water-level declines are so large near the presumed pinchout of the Bucatunna to the east suggests that some degree of confinement of the undifferentiated Floridan aquifer may prevail, in contradiction to assumptions accepted as a basis for the model. This area is about 45 miles east of injection site 2 and about 30 miles east of regional monitor well 1. Based upon findings of the image well analysis, misrepresentation of the position or hydraulic character of this boundary or changing local water levels would have a negligible effect upon computed water-level changes at the injection sites during the simulation time period, though there could be a slight influence upon water-level changes computed for regional monitor well 1.

The changing water levels east of Fort Walton Beach would have little significance for the prestress regional flow simulation. However, they could have an appreciable effect upon the simulated regional flow system caused by injection, as they represent a hydraulic influence during the simulation time period not represented in the model. The falling water levels represent the hydraulic influences of both the pumping stress and of any degree of confinement which exists within the cone of influence of the pumping beyond the eastern limit of the Bucatunna. An assessment of the effects upon the southeastern part of the regional flow simulation follows in a subsequent section.

In the southeastern part of the modeled region, from the Bucatunna pinchout near the center of Choctawhatchee Bay southward, no data describing the injection zone or its degree of confinement were available. It was assumed that the eastern pinchout of the Bucatunna continued southward to the probable location of a Gulf of Mexico subcrop, and that a constant-head representation was appropriate. A constant-head boundary was also assumed for the southern subcrop boundary. A water-level value of 0 foot was assigned to subcrop boundaries. This was too low, as the equivalent freshwater heat 1,600 feet beneath the surface of the Gulf of Mexico would be 41 feet, and 77 feet would be the equivalent freshwater head at 3,000 feet. The two depths bracket the unknown, and likely varying, depth of the injection zone subcrop. A further complication to the assignment of water-level boundary values is the possible presence of saltwater in the aquifer inland north of Choctawhatchee Bay.

As previously stated, if steady initial conditions were used, erroneous specification of water levels at a constant-head boundary such as the Gulf subcrop would not affect the computed water-level changes, by linearity of the differential equation for flow. They could, however, appreciably distort the southeastern part of the regional flow simulation used as an initial condition. The regional flow simulation could also be distorted with unknown effect if constant-head boundaries representing a pinchout underneath the Gulf or the subcrop were not properly located, or if the aquifer were inappropriately described as unconfined when it is at least partially confined. Such mischaracterization of conditions at southeastern and southern boundaries would not much affect water-level changes computed at control points because of the large intervening distance (at least 50 miles).

The needs for additional information to adequately describe aquifer conditions to the east and south of the study area is highlighted by these considerations. Besides adequate descriptive data, incorporation into the model of the effects of upper limestone pumping or the presence of confining layers above the Bucatunna would probably require a multilayer or three-dimensional approach.

Simulation of Prestress Regional Flow System

The location and type of boundaries for the model of the flow system having been decided upon, subject to some reservations, it was decided to use the areal distribution of transmissivity from corresponding parts of the infinite aquifer simulation. Thus, simulation of the regional pre-injection water levels required the adjustment of the remaining set of parameter values, the hydraulic head values along the constant head boundaries, all other boundaries being zero-flux. Water-level data control was scanty for a selection of constant boundary head values, so guidance was sought from a survey of geohydrologic field studies in southern Alabama and Okaloosa County, Fla.

Previously cited water-level values of 128 feet, measured in 1961 at regional monitor well 3, and 137 feet, measured in 1968-69 at another injection zone well in Escambia County, Ala. (M. E. Davis, oral commun., 1977), were considered. Davis also reported another Ocala Limestone water level of 243 feet above sea level (1965-78) to the north in southeastern Conecuh County, Ala. An average value of 350 feet above sea level was measured in 1959 and 1960 in the Eocene and adjacent layers near Monroeville in Monroe County, Ala. (O'Rear, 1964). Powell and others (1973) reported a water level of 129 feet above sea level at the Pollard oil field, 13-14 miles west of regional monitor well 3, in the Marianna Limestone, the unit overlying the injection zone in this area. Cagle and Floyd (1957) reported a range of 80-100 feet from the Brewton area of Escambia County, Ala., which seemed anomalous compared to the other values.

Water levels assigned to model boundaries corresponding to locations to the northeast of the study area, in Okaloosa County, Fla., and to the east of the study area, near the boundary of Okaloosa and Walton Counties, were based upon a generalized 1942 potentiometric surface of the upper limestone of the Floridan aquifer and the upper part of the undifferentiated Floridan aquifer (Trapp and others, 1977). These water levels, obtained when wells were drilled for Eglin Air Force Base water supply and predating large municipal withdrawals for the city of Fort Walton Beach, were also considered representative of conditions in the lower limestone, including the injection zone, wherever the intervening Bucatunna Clay Member was absent. South of Choctawhatchee Bay, where a continuation of the pinchout of the Bucatunna was presumed, constant head value assignments decreased southward from the values used in southern Walton County. Constant head value assignments were to the nodal centers of large grid cells included just within the constant head boundary indicated in figure 8. Zero-flux boundary grid cells lie just outside the indicated boundaries on all sides of the figure. The grid design in the center of the modeled region was the same as for the infinite aquifer simulation (table 1).

Only minor adjustments had to be made to initial boundary value estimates to make the computed preinjection water level at the first Monsanto Company injection well (site 1) agree with the measured one. Agreement was good at the two other preinjection control points. The resultant pattern of water-level contours (fig. 8) in the study area was similar to that of the data-based contours (fig. 7), and supported the interpretation of a southeasterly flow regime oriented 70° to 80° counterclockwise from the downdip direction of the aquifer.

Nevertheless, it is evident that the simple three-strip uniform transmissivity distribution and the boundary assumptions provide only a highly generalized simulation of the injection zone in the study area. The previously cited large water-level difference between the deep test monitor well (site 2) and regional monitor well 1 is not portrayed. The computed and reconstructed prestress water-level values at the former differ by 5 feet, but the values at the latter differ by 20 feet. As no data were available to verify that transmissivity variations caused this discrepancy nor to describe the nature of the variations, any effort to simulate them would only have been of hypothetical interest, so this was not done.

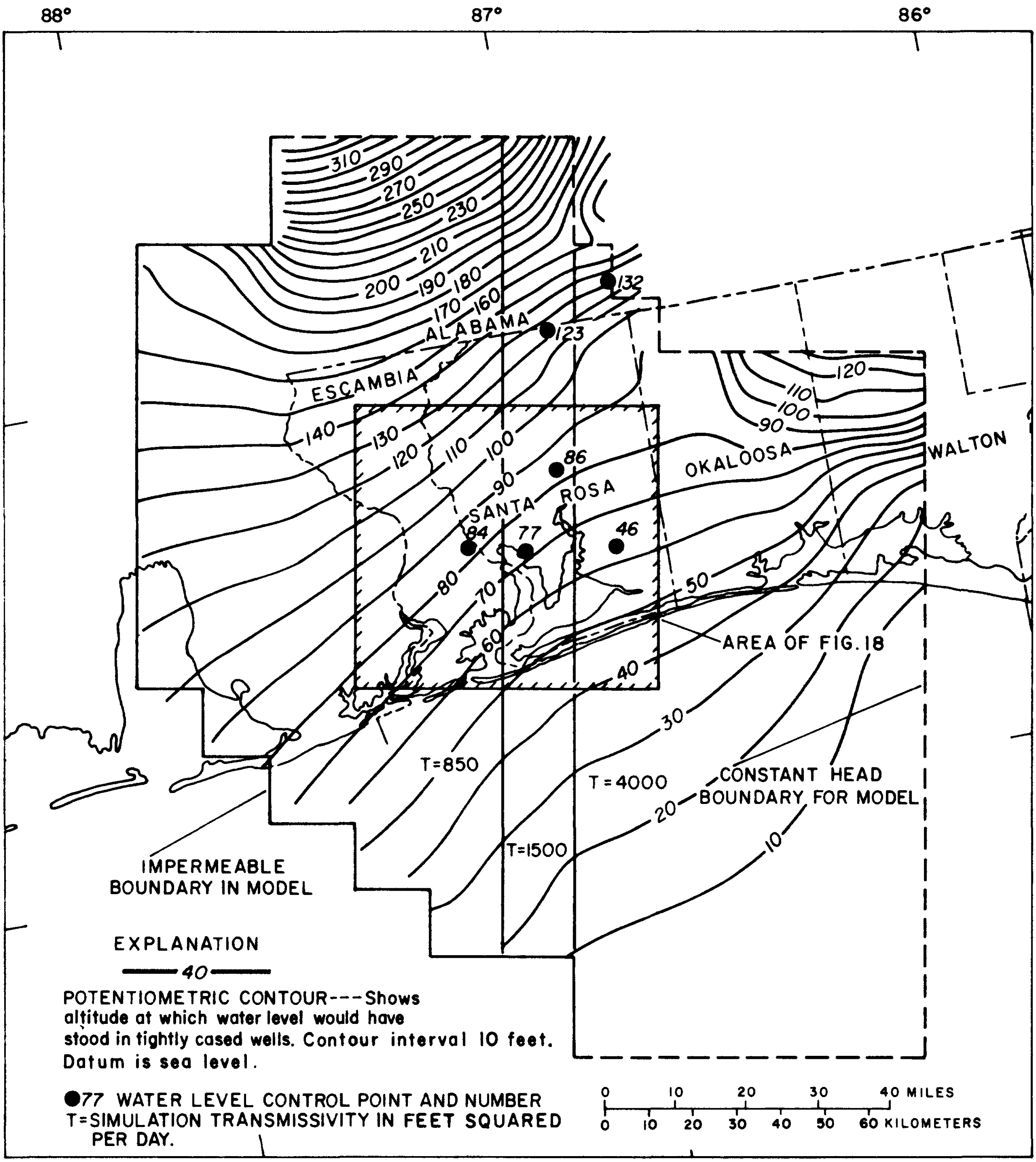

Figure 8.--Computed preinjection water levels from steady-state two-dimensional flow model simulation incorporating natural aquifer boundaries.

The 6-foot decline of water levels near the northeastern boundary was probably slight enough that the effect on flow across the boundary would be negligible. The 30-40 foot decline at the eastern pinchout of the clay would cause somewhat greater discharge to occur in this area and a slightly more eastward orientation of the natural flow system than shown by the model. Specification of higher water-level values along the subcrop boundary and where saltwater penetrated inland would also tend to shift discharge toward the midpoint of the eastern boundary, and perhaps eliminate simulated discharge across the subcrop boundary. A no-flow boundary might have been appropriate for these sections. Though the southeastern part of the depicted flow system is known to be distorted, additional (but unavailable) data would have been required for accurate refinement of the simulation, so no further efforts were made.

Figure 8 shows a relatively uniform spacing of potentiometric contours about the two injection sites prior to injection (water levels are with respect to 5,000 mg/L of dissolved solids). The water-level gradient at each site is shown to be southeast: 1 foot of altitude in 2,400 feet at injection site 1, and 1 foot of altitude in 3,000 feet at injection site 2. Using the calibrated site 1 transmissivity of 850 ft^2/d, and assuming porosity to be 28 percent and layer thickness 60 feet, the local water particle velocity (Darcian velocity divided by porosity) from natural regional flow would be about 8 ft/yr. The porosity and thickness values are suggested from an interpretation of data at injection site 2 (Ehrlich and others, 1979). Using the calibrated transmissivity of 1,500 ft^2/d at the latter site, local water particle velocity would be about 11 ft/yr.

Simulation of Water-Level Changes

Using the same parameter values, the transient response of the aquifer to injection stress was also computed with the natural boundaries represented in the model. Water-level response curves were similar to those computed when the northeast boundary was simulated with an image well. This was an expectable result as the northeast boundary was the only one shown to have an appreciable effect on water-level changes at any of the observation wells. At most monitor well locations, water-level changes in the two solutions did not differ by more than a foot. The only exception was regional monitor well 3, where the image-well simulation showed a water-level rise of 2 feet by October 1978, but the natural boundary simulation showed a rise of 7 feet. This difference, and slighter differences at the two regional monitor wells, are likely due to the different method of representing the location of the northeast boundary, estimated to be in near proximity to regional monitor well 3.

A cumulative water budget was computed for the part of the injection zone within the model boundaries. By August 31, 1977 (after 5,175 days of injection at site 1 and 822 days of injection at site 2), 1.95×10^9 ft^3 of liquid waste had been injected. Pressures from the injection created 1.29×10^9 ft^3 of additional storage for the waste within the section of aquifer enclosed by the model boundaries, by compression of the aquifer material and of the fluid itself. This seems large, but is actually negligible compared to the total volume of water (4.74×10^{12} ft^3) within the large area enclosed by the model boundaries. There was 2.16×10^9 ft^3 of inflow from recharge areas, 2.82×10^9 ft^3 of outflow across discharge boundaries, and the net discharge across boundaries was 0.66×10^9 ft^3.

Because of the combination of effects of local and distant hydraulic characteristics on the water levels at a given control point, and because of the sparse areal distribution of measurements of hydraulic characteristics and of water-level control points, calibrations based upon the three-strip parameter choices did not prove these choices correct even at the water-level control points where aquifer characteristics were measured. The valid result of the analysis was the simulation of water-level changes and the generalized simulation of preinjection water levels at the control points.

SWIP Simulations of Regional Flow System and Water-Level Changes

The final step in the analysis of hydraulic effects of injection was the replication of the two-dimensional flow model steady-state and transient solutions with the more sophisticated SWIP model. The time-invariant boundary representation of SWIP differs from that of the two-dimensional flow model in the location of the point at which conditions are considered constant, approximately at the midpoint of the outer boundary of the boundary grid cells. Nodal values at the centers of boundary grid cells remain dependent variables of the computations. This required removal of no-flow and constant head grid cells from the outer boundary of the two-dimensional flow model grid, redimensioning of the new outer grid cells, and some adjustment of the constant head values. The omission of any specification of conditions at an outer boundary was equivalent to a zero-flux (no flow) specification. The internal grid design of the flow model simulations was retained except for minor redimensioning about the position of injection site 2. This was to incorporate in-situ measurements of distances between wells by adjusting the spacing between the corresponding nodes. Previously, distances between wells had been back-computed from geodetic coordinates. The resultant effect upon computed water-level changes appeared to be negligible.

A concentration value (C=0) was assigned uniformly to the native aquifer water throughout the entire region modeled, consistent with the conversion of all observed water levels to a common salinity standard (5,000 mg/L of dissolved solids). C=1 was the concentration value assigned to the injected fluid. Corresponding density assignments, 62.71 lb/ft^3 (C=0) and 62.52 lb/ft^3 (C=1), did not affect the regional hydraulic solution. Minor effects on water levels within the range of waste transport near the wells will be discussed further on.

The three-strip transmissivity distribution was virtually the same as that of the two-dimensional flow model simulations, but was entered as a combination of layer thickness and intrinsic permeabilities at specified conditions of temperature, pressure, and solute concentration. A slight areal variation was introduced by the SWIP dependence of hydraulic conductivity upon density, related in turn to injection-zone pressure, which varied appreciably within the modeled area because of the aquifer dip. An estimate of aquifer storativity was not needed for the steady-state simulation. The temperature of the native aquifer water was assumed to range from 92°F to 93°F in a 60-foot interval below the top of the injection zone, approximately the thickness of the most permeable part of the zone as estimated from fluid-velocity logs from injection site 2. The effect of this slight gradient upon computed water-level changes was negligible.

Setting pore volume equal to a very small value at all grid nodes within the constant pressure and zero flux boundaries, SWIP was run for seven iterations, in which it converged to a very close approximation of steady-state. The resulting simulated preinjection water-level distribution in the injection zone (fig. 9), was very similar to that computed by the two-dimensional flow model simulation incorporating natural boundaries (fig. 8). Slight differences, due to pressure-related density variation and concomitant minor variations in the SWIP hydraulic conductivity parameters, increased toward the northeast, in the aquifer updip direction in which pressure decreased. These differences ranged from 0.1 foot at the site 1 north monitor well, to 2.1 feet at the deep test monitor well (site 2) and regional monitor wells 1 and 2, and to 5.5 feet at regional monitor well 3 near the Alabama border.

A representation of aquifer storage properties was required for the SWIP transient simulation of water-level response to injection stress. The SWIP representation of storativity is based upon the relationship with porosity, layer thickness, water and rock compressibility, and aquifer water density described by Lohman (1979). An areally uniform estimate (28 percent) of the effective porosity of the upper, most transmissive part of the injection zone was based upon the sample from injection site 2 (Pascale, 1975). Assuming the native water to have a density of 62.55 lb/ft^3 (C=0 value adjusted to aquifer temperature and pressure conditions at the site), it was found that a porosity value of 28 percent, a permeable zone thickness of 59.5 feet, and a value of $3.5x10^{-5}$ in^2/lb for the compressibility of the aquifer material were equivalent to the storage coefficient of $2.75x10^{-4}$ used in the two-dimensional flow model. Any other combination of these coefficients equivalent to a storage coefficient of $2.75x10^{-4}$ would also have produced the same water-level changes in SWIP computations, so the choices were not of major significance for the hydraulic simulation. Their significance for the waste transport calculations will be discussed later. Since density exhibited a slight areal variation in the SWIP computations by virtue of its dependence upon pressure, which varied near the injection sites owing to injection stress and across distances owing to the dip of the aquifer, and consequence increase in pressure downdip, the SWIP equivalent of the storage parameter was not quite areally uniform.

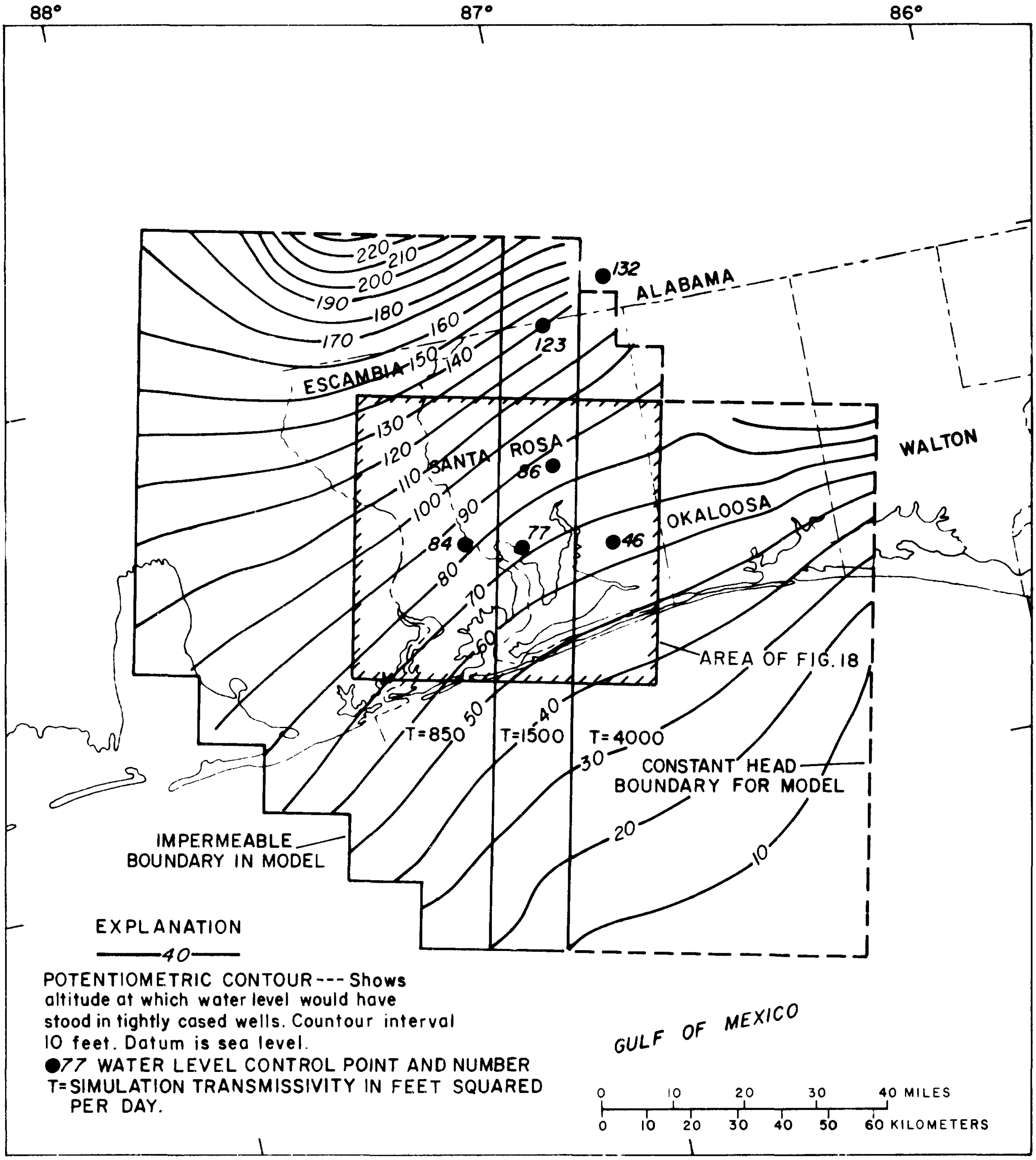

Figure 9.--Computed preinjection water levels from steady-state SWIP simulation.

The discretization of average injection rates (figs. 2, 3) used in the two-dimensional flow model runs was retained unchanged. The hydraulic response to 15 years of injection stress was computed and the then future response in 1980 to 1978 injection rates was predicted. Water-level changes were very similar to those of the two-dimensional flow model simulation with natural boundaries. Minor differences near the injection wells were attributable to density effects related to the computed arrival of the injected fluid at observation wells.

Computed and observed water levels are illustrated in figures 10 through 16. Figures 10 and 12 show two-dimensional flow model output and corresponding curves from sensitivity analyses. The remaining figures show SWIP output. The "observed data" differ from actual measured water levels by the adjustment to 5,000 mg/L of dissolved solids and by adjustment to sea level. To obtain the measured values, they should be corrected by the suggested factors and adjusted to land surface datum. The computed curves have been arbitrarily shifted as a means of superposing observed and computed curves to better show the lack of cumulative bias or amplitude errors in the computed data. It is not possible to reference both curves to prestress initial values, as preinjection water levels were not measured at most control points and were not accurately simulated by the regional flow model. The shifting was done on the basis of the average of signed differences in a time series of corresponding computed and observed (adjusted) water-level values (the time points where computed values are shown in figs. 10 through 16).

Some differences between computed and observed values are evident. At the north and south monitor wells near injection site 1, computed values are consistently lower throughout much of 1973 (figs. 10-11). The reason for this is unknown, as reported monthly average injection rates were not consistently larger than the long-term simulation rates. Prior to the commencement of injection at site 2 in 1975, simulated water levels from the nearby deep test monitor well (fig. 12) seem to show a slight cumulative negative bias (about 3 feet in 3 years during which the total water-level increase was about 80 feet). However, after 1975, computed and observed water-level curves seem to match, as do the curves from the nearby standby injection well and north monitor well (fig. 13). It is more difficult to compare deep test monitor well water levels in this later time period as measured data oscillate considerably in response to short term rate variations at the nearby injection well.

The largest deviation between computed and observed water-level curves occurs at the location of regional monitor well 3 (fig. 16, which only shows years when water levels were measured). Computed water levels from 1963 to 1978 show a gradual rise of 5 feet, whereas observed water levels declined 13 feet. This well was very close to the estimated limit of the Bucatunna and water levels at this location were influenced by those in the unconfined upper Floridan. The 6-foot decline at the U.S. Geological Survey observation well in Alabama indicates the lowering of unconfined water levels in the region.

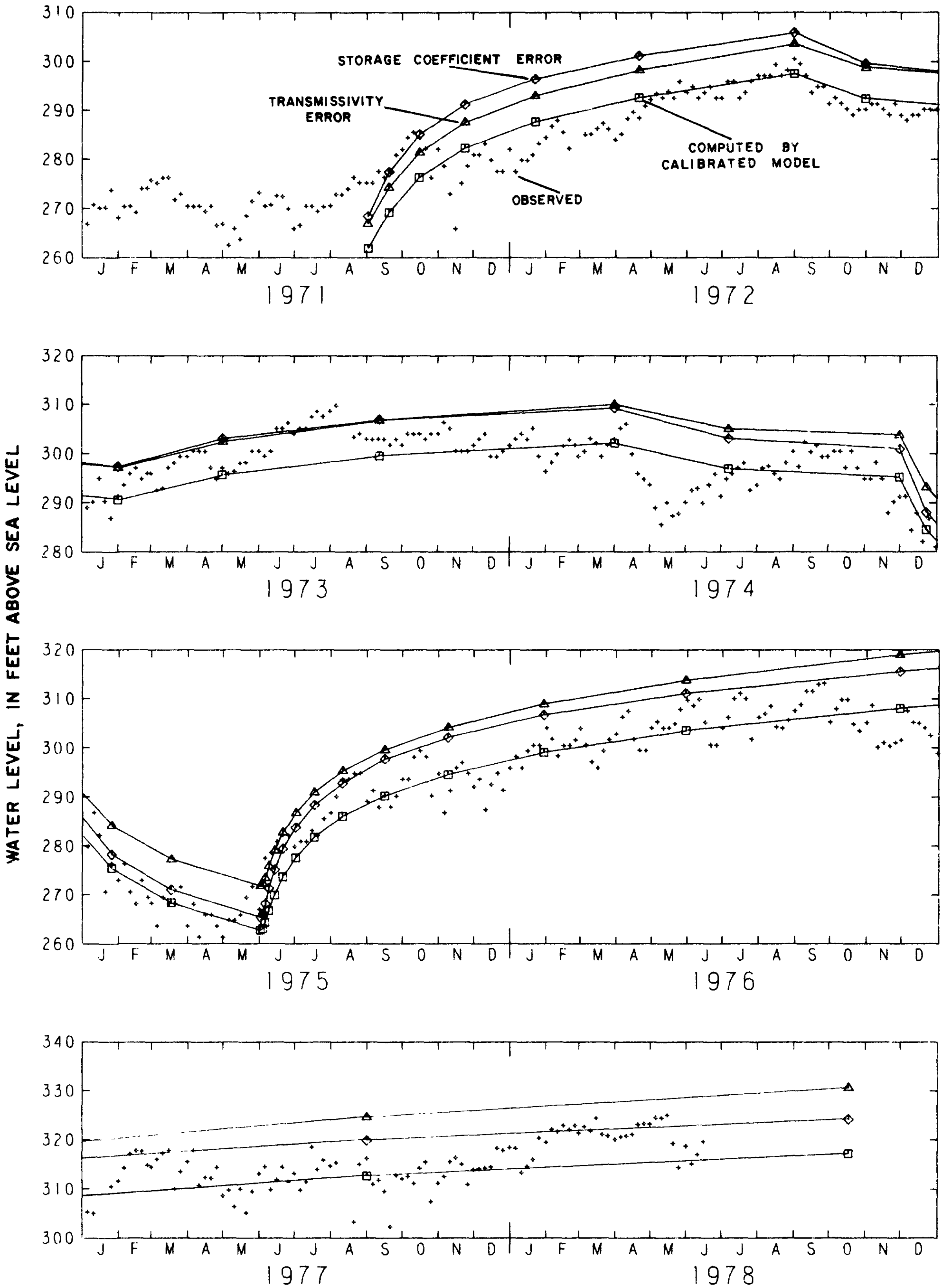

Figure 10.--Observed and computed water-level changes at the south monitor well, injection site 1. Computed by two-dimensional flow model. Land surface datum is 15.2 feet above sea level. The salinity correction factor was +8.5 feet till August 1977 and +5 feet afterward. The average deviation was -1.4 feet. The computed curve was not shifted.

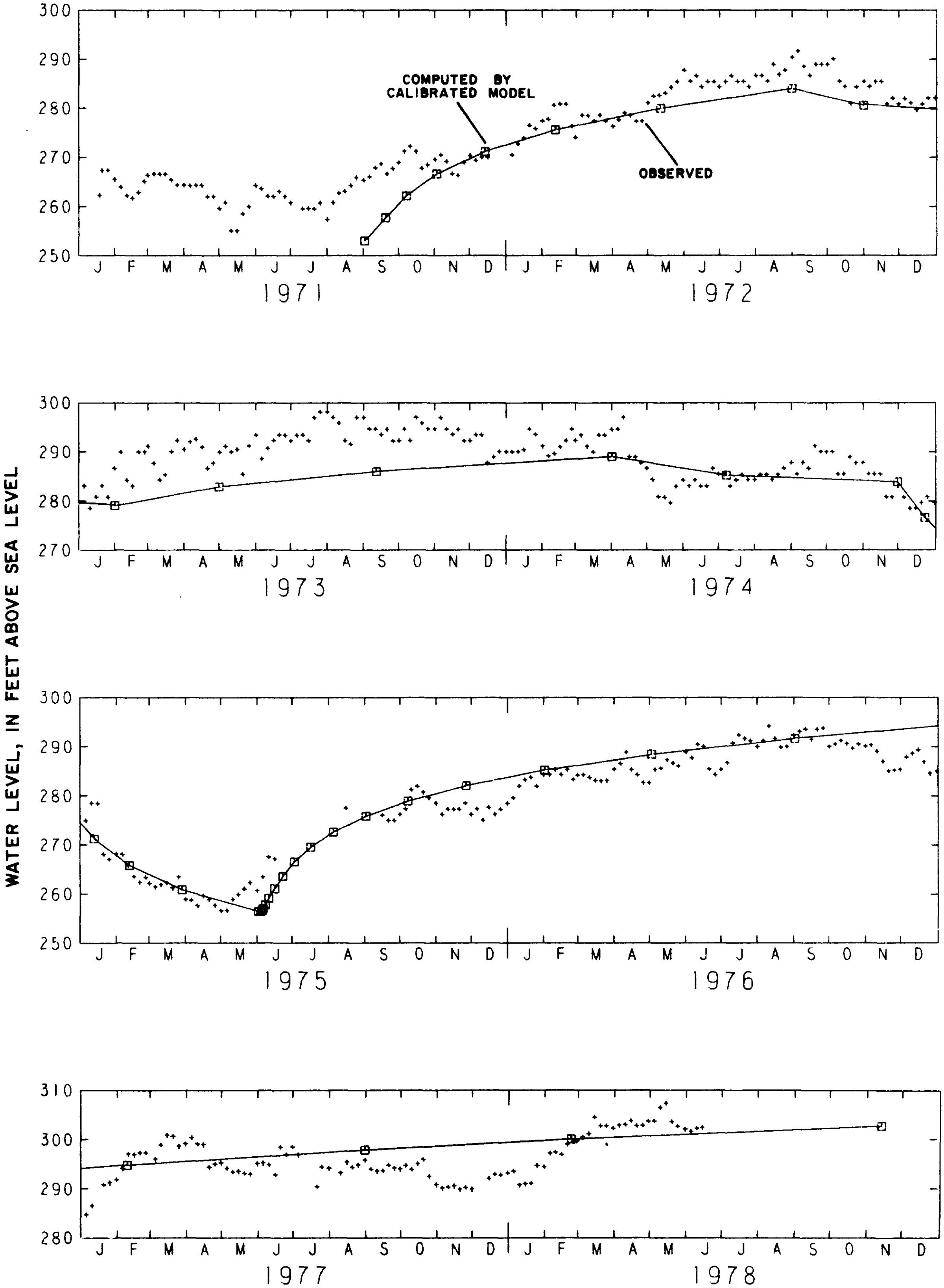

Figure 11.--Observed and computed water-level changes at the north monitor well, injection site 1. Land suface datum is 7.8 feet above sea level. Salinity correction factors were +5 feet to December 1971, +10 feet to August 1977, and +5 feet afterward. The average deviation was -4.9 feet. The computed curve was shifted +2 feet.

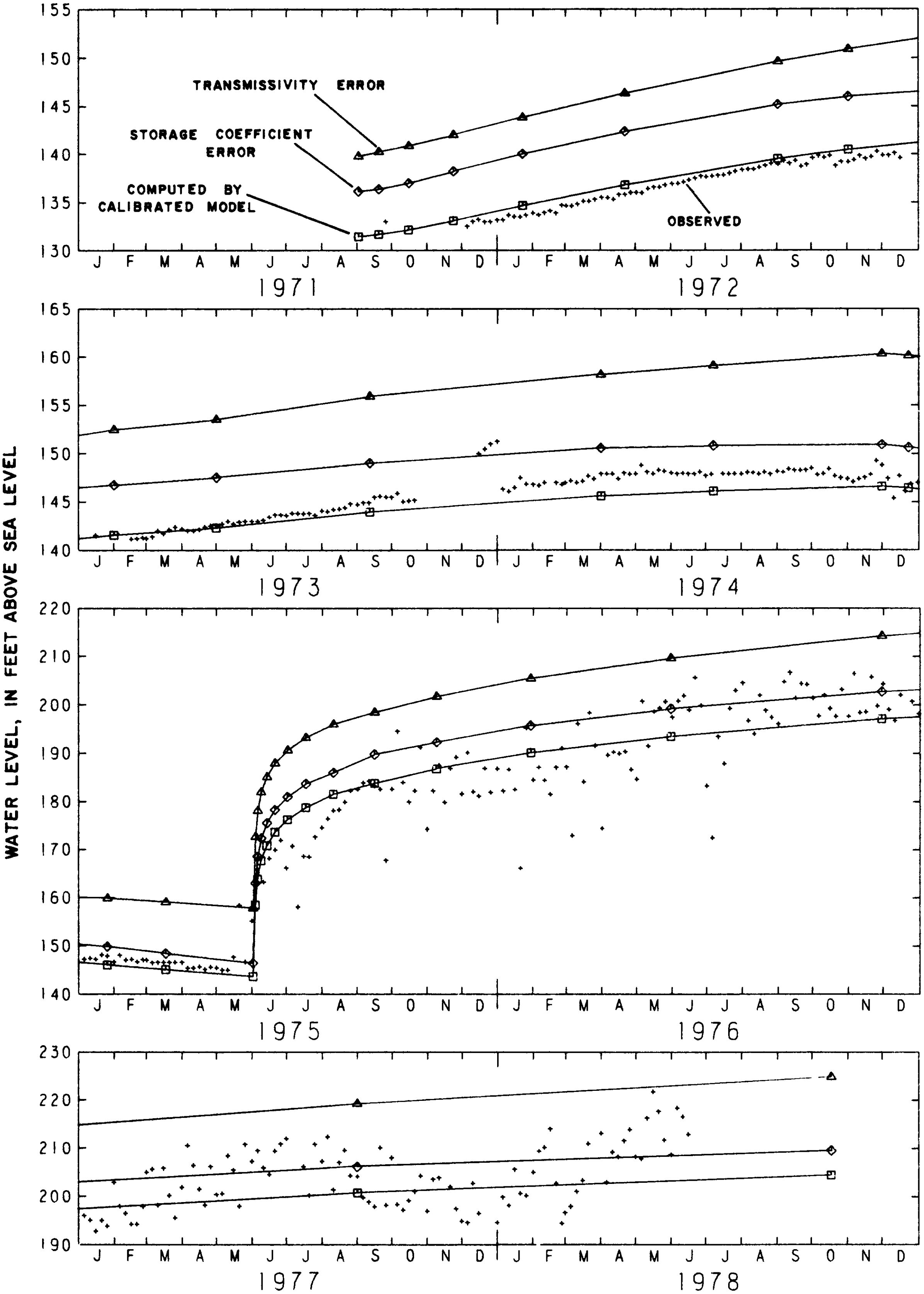

Figure 12.--Observed and computed water-level changes at the deep test monitor well, injection site 2. Computed by two-dimensional flow model. Land surface datum is 101.5 feet above sea level. Salinity correction factors were +1 foot to January 1973, +5 feet to January 1974, 0 foot to August 1976, and -1 foot afterward. The average deviation was -4.1 feet. The computed curve was shifted +4 feet.

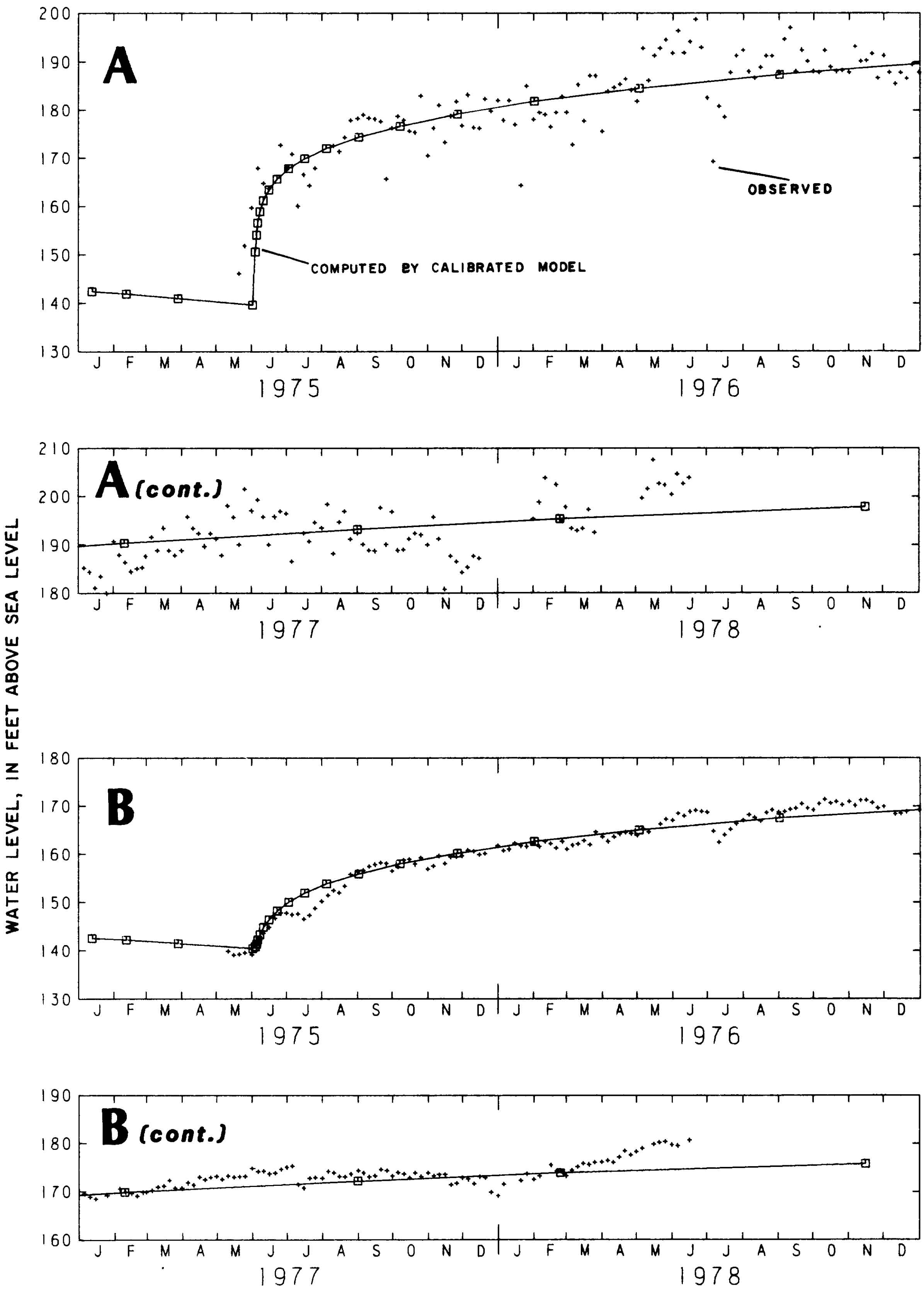

Figure 13.--Observed and computed water-level changes at two injection site 2 monitor wells. At the standby injection well (A), land surface datum is 68.4 feet above sea level. Salinity correction factors were +8 feet to July 1976 and +4 feet afterward. The average deviation was -1.3 feet. The computed curve was shifted by +1 foot. At the north monitor well (B), land surface datum is 121.9 feet above sea level. The salinity correction factor was -1.5 feet. The average deviation was -5.3 feet. The computed curve was shifted +6 feet.

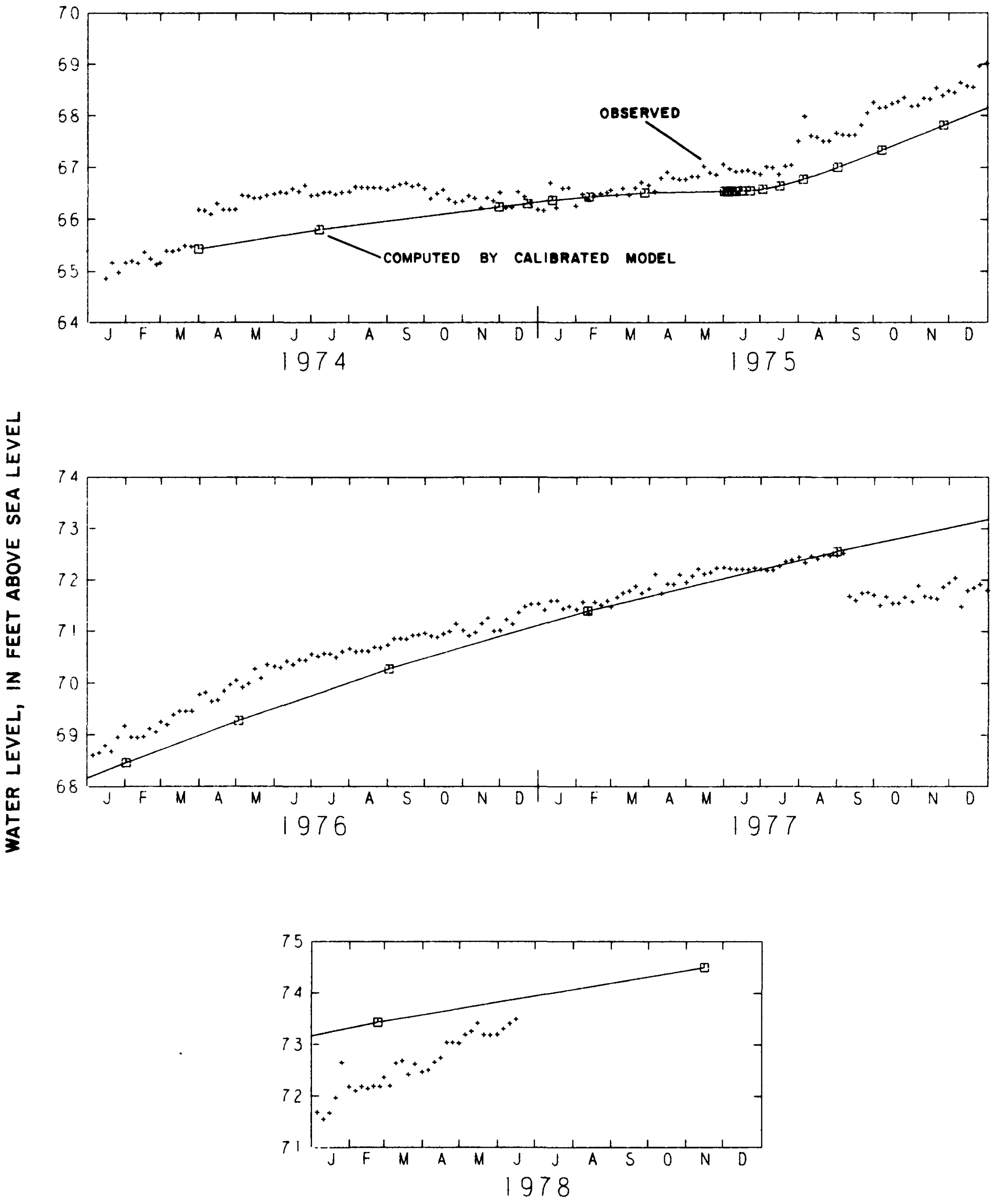

Figure 14.--Observed and computed water-level changes at regional monitor well 1. Land surface datum is 125.4 feet above sea level. The salinity correction factor was 0 foot. The average deviation was +19.7 feet. The computed curve was shifted -20 feet.

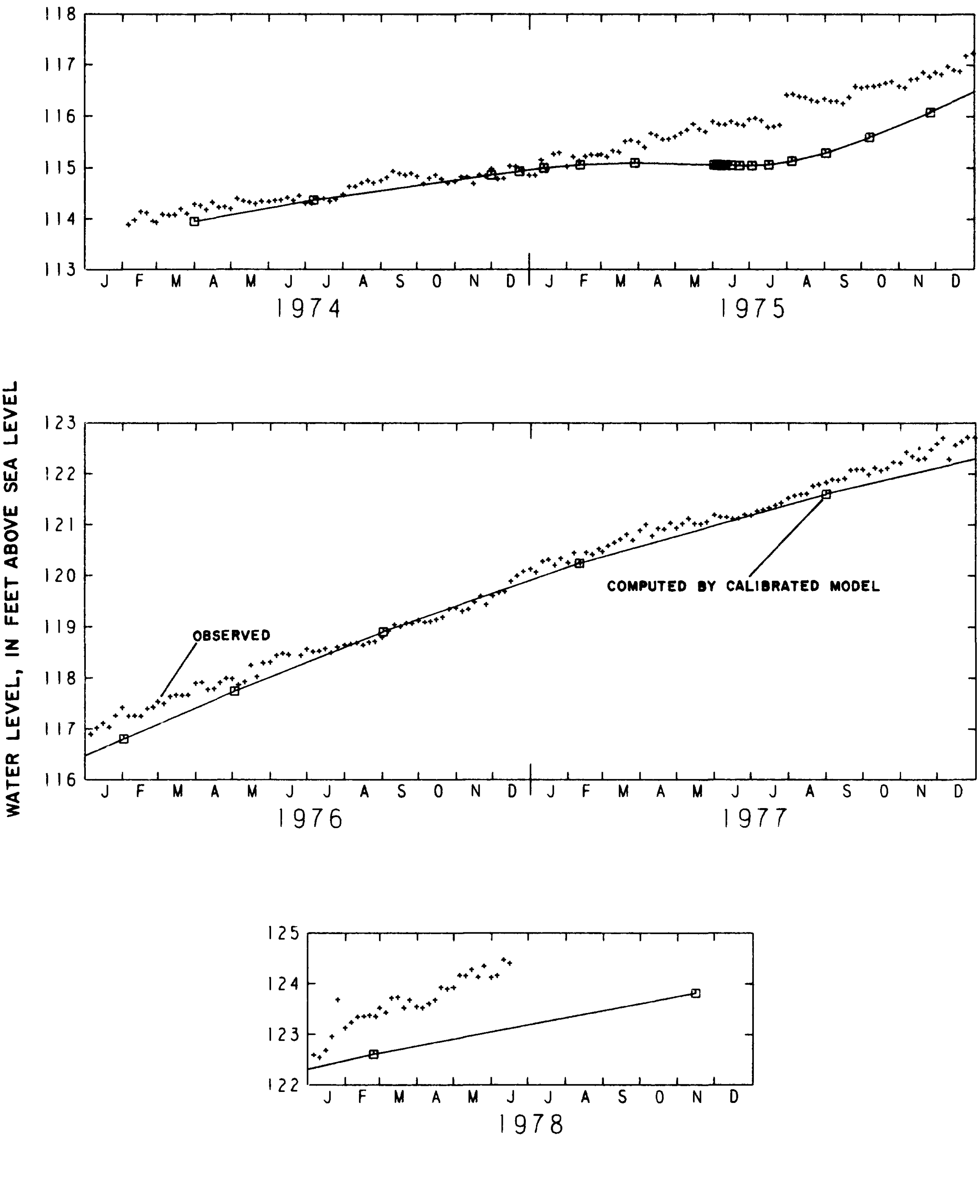

Figure 15.--Observed and computed water-level changes at regional monitor well 2. Land surface datum is 125.0 feet above sea level. The salinity correction factor was -4 feet. The average deviation was -2.3 feet. The computed curve was shifted +2 feet.

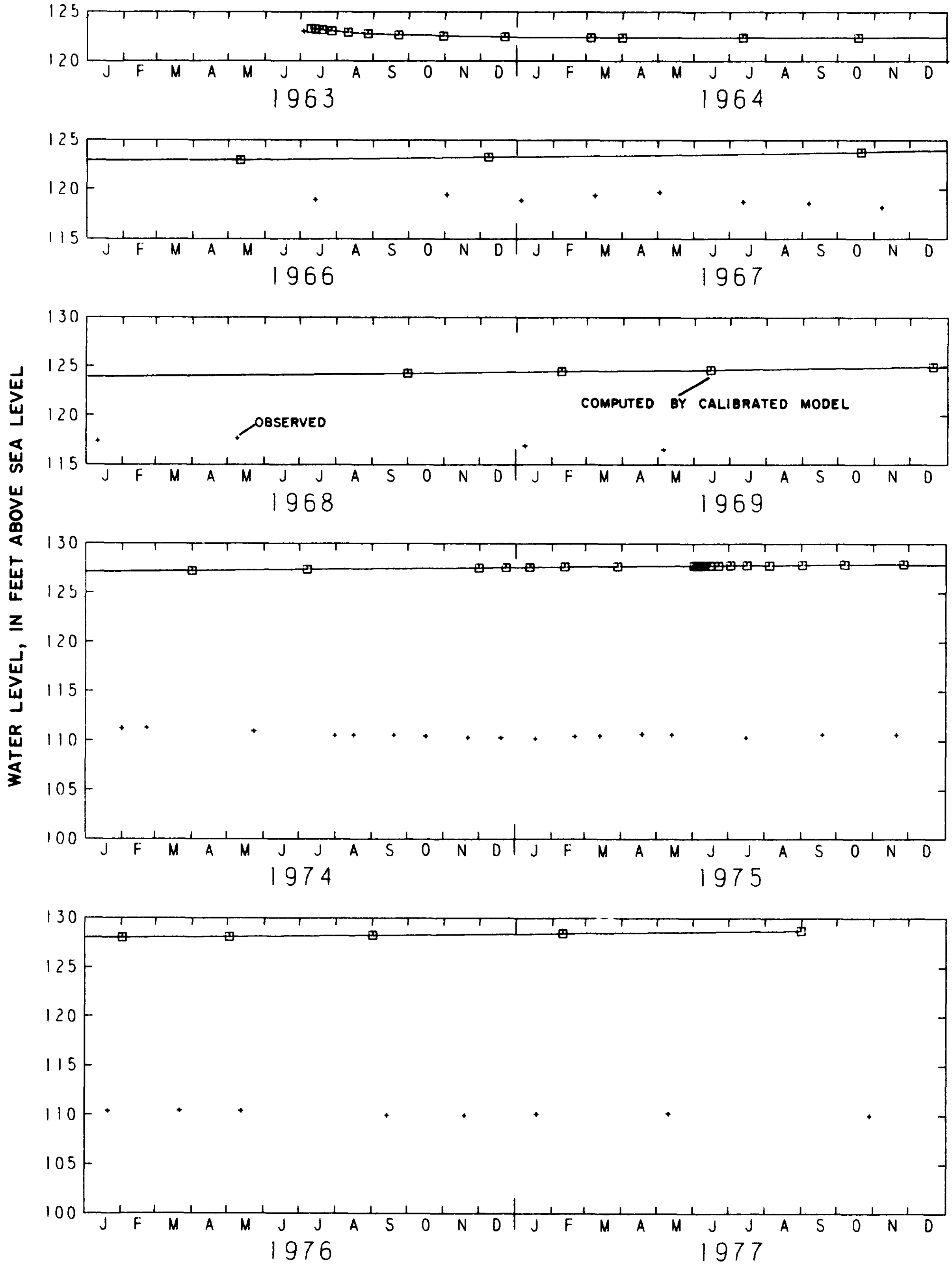

Figure 16.--Observed and computed water-level changes at regional monitor well 3. Land surface datum is 280.0 feet above sea level. The salinity correction factor was -5 feet. The average deviation was 24.3 feet. The computed curve was shifted -8.5 feet so that initial water levels would coincide.

There are also minor differences immediately before and following the simulation times corresponding to changes in the long-term average simulation injection rates. This is because actual rate changes were more irregular and gradual. In particular, the beginning of injection on a regular basis at each site was preceded by several injection tests which raised local water levels prior to the beginning dates used for simulation.

The computed water levels in all or part of the region enclosed within the model boundaries were contoured at selected times during the injection history (figs. 17 and 18). These contours represent the superposition of computed water-level changes upon the generalized regional flow system (fig. 9). They are useful in showing qualitatively the regional flow regime resulting from injection stress, but should not be used for detailed interpretation. Contours outside areas of data control are unverified due to the lack of information about aquifer characteristics, and contours in areas of data control may have biases of 5 to 20 feet owing to inaccuracies in the computation of steady-state initial conditions. Contours near the eastern and southeastern (subcrop) boundaries are suspect because of lack of information about the extent and degree of confinement, because simulated subcrop boundary water levels were too low, and because the drawdowns from Fort Walton Beach pumping were not simulated. Water levels shown are with respect to 5,000 mg/L dissolved solids, not the actual local salinity, but do not contain the arbitrary "shift" of figs. 10 through 16.

Figure 17 shows simulated conditions for August 1977 in the entire modeled region. Other illustrations (fig. 18a-e) show water-level contours in a 43-mile by 40-mile area about the two injection systems (hachured outline in the center of fig. 17) at various times: September 1971, November 1974, June 1975, August 1977, and June 1980. The June 1980 contours project 1978 average injection rates. All plots omit contours of values higher than 200 feet above sea level, even when model computations show such higher water levels over a sufficiently large area about site 1 to be clearly portrayed. This is because computed wellhead water levels at the single well used to simulate site 1 injection and ones measured in the two actual site 1 injection wells show considerable disagreement. This may partly owe to the fact that the two wells were actually 1,300 feet apart.

That measured water levels in the wells at site 1 are much less than the computed ones also likely owes in part to the gradual solution of aquifer material about the wells by the strongly acidic injectant and the resultant local increase in hydraulic conductivity, which was not represented in the model. The hydraulic effects of solution are assumed to be restricted to a small enough area that monitor well water levels (at least 1.5 miles away) have not been affected. As the purpose of the study was to simulate regional effects of injection, attempts to simulate water levels close to the injection wells were beyond its intended scope. SWIP has the potential for such an application, however, if consideration is given to a host of new problems (well losses, conductivity/porosity relationships, and so forth) not treated in this study.

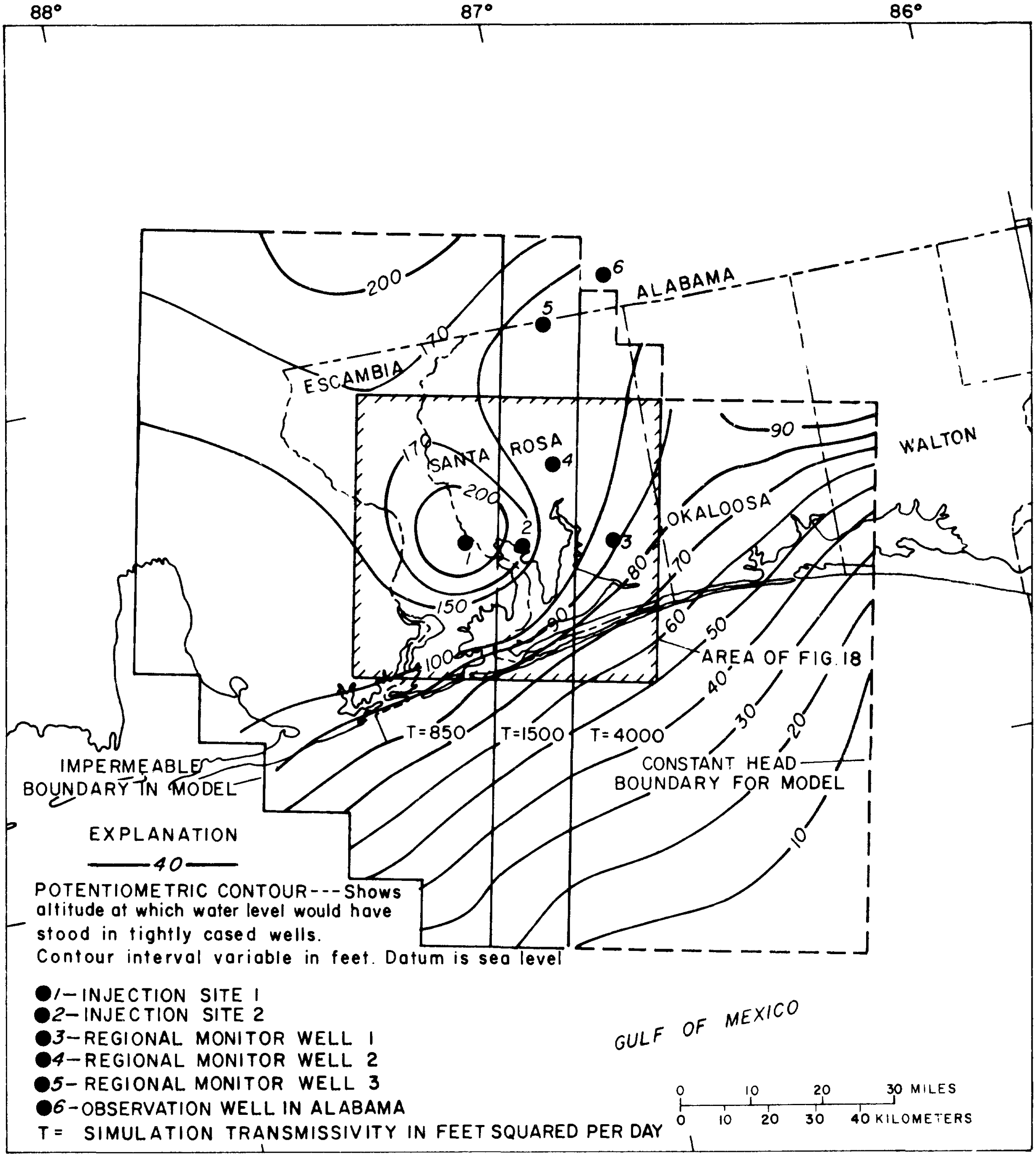

Figure 17.--August 1977 water levels from SWIP simulation.

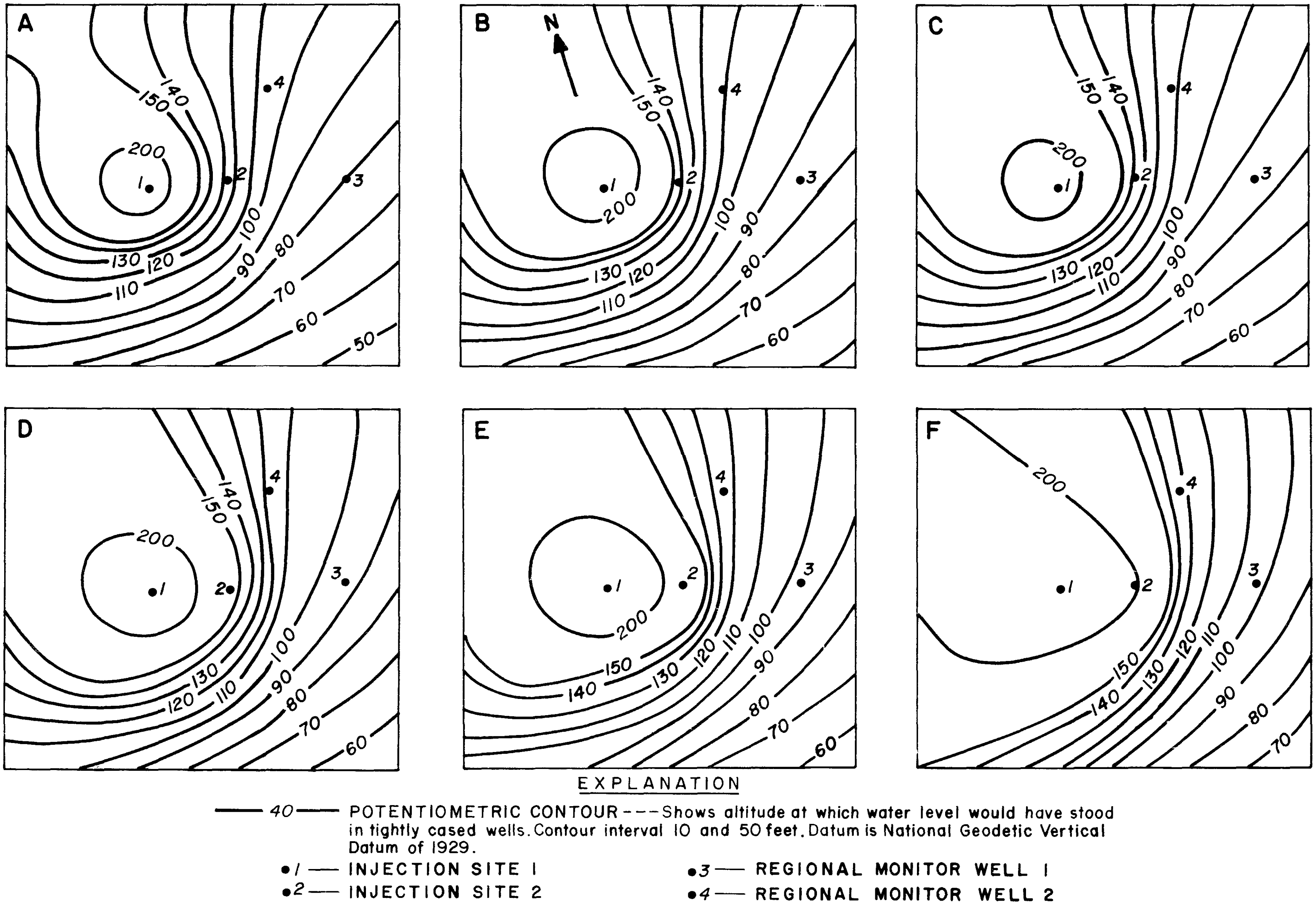

Figure 18.--Water levels in an area about the injection sites computed for various historical and future simulation times. The times shown are: A - 2,984 days (9/1/71), B - 4,170 days (11/30/74), C - 4,353 days (6/1/75), and D - 5,175 days (8/31/77). E is a projection for 6,206 days (6/27/80) on the basis of 1978 rates, and F shows the ultimate equilibrium steady-state resulting from the continuation of injection at 1978 rates. A - C show the effect of injection at site 1 only; the remaining figures show the combined effect of injection at both sites.

The June 1975 contour plot shows lower water levels than the November 1974 plot, a result of the very low average injection rate at injection site 1 during the intervening time period. The August 1977 and June 1980 plots show the 200-foot contour encircling injection site 1 to have a slight bulge in the direction of injection site 2 where waste injection at a lower average rate for a shorter duration had generated a smaller pressure mound than at injection site 1. There was actually a small area around injection site 2, too small to illustrate, with simulated water levels in excess of 200 feet. By mid-1978, the computed water-level change at the primary injection well (site 2) was about 108 feet. Data (Hull and Martin, 1982, p. 15) show an average wellhead pressure increase in the range of 27 to 44 lb/in^2, equivalent to a water-level increase of 62 to 101 feet, in the first half of 1978. Again, no attempt was made to improve the computation of water levels close to the injection well.

Ultimate Hydraulic Response to Injection at 1978 Rates

The response of water levels to injection at 1978 rates at the two sites was projected into the infinite future when the water-level distribution in the aquifer would reach an equilibrium determined by natural aquifer flow and injection outflow. This was accomplished by allowing SWIP to iterate to steady-state with pore volume set equal to a very small value and with current injection rates specified. Figure 19 shows equilibrium water-level contours in the region enclosed by model boundaries, and figure 18f shows them in a 43 by 40-mile area about the injection sites. Water levels 200 feet above sea level and higher are shown to extend throughout the entire region between the injection wells, and the 200-foot contour is open to the northwest.

Neither the differences between the 1980 and equilibrium flow regimes nor the differences between the 1977 simulation (fig. 17) and equilibrium are major, indicating that the flow system was approaching steady-state under current injection rates in 1978. However, a comparison of 1977 and equilibrium contours shows flow to be more easterly in the latter. This is because water levels continue to rise after 1977 near the western and southwestern impermeable boundaries, but rise more slowly near the (unconfined) recharge boundaries to the north where water levels are considered to remain approximately constant. Qualifications concerning the contours portrayed in the southeastern part of the modeled area continue to apply.

Sensitivity Analyses

Sensitivity analyses are often performed at stages in the calibration of a simulation model in order to determine the degree to which perturbations in parameter specifications or grid design affect the computed dependent variables. Results can be used to evaluate the adequacy of the data base and the need for data of greater or less precision. Although guidelines exist for the structuring of sensitivity analyses for ground water models, no absolute rules are justified in theory, and sensitivity analyses are best designed to provide insights of significance within the framework of a particular study.

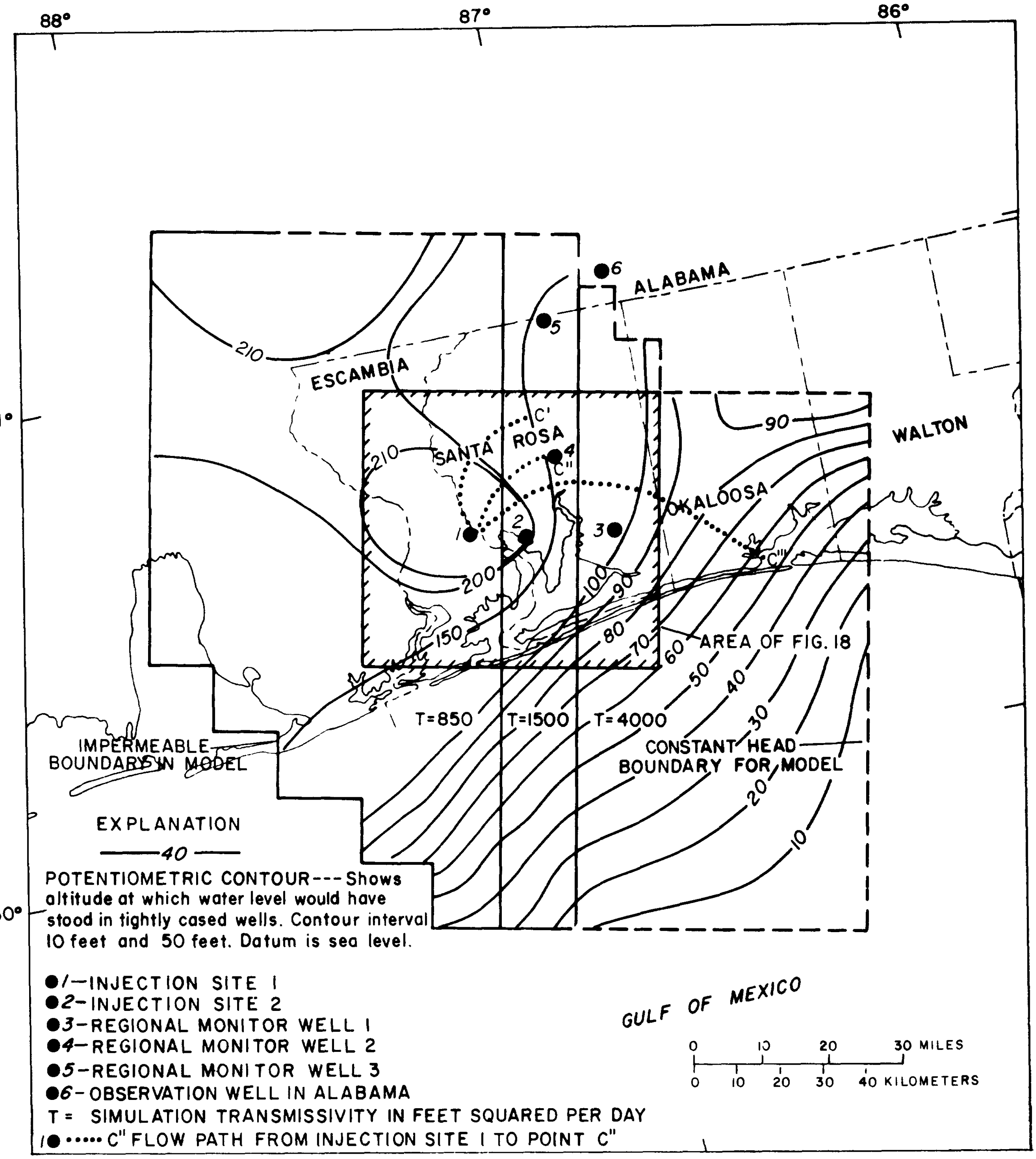

Figure 19.--Water levels from SWIP simulation showing the result of an infinite continuation of injection at 1978 rates.

The three vertical strip transmissivity value distribution of 850, 1,500, and 4,000 ft^2/d of the calibrated model was used as a control for one set of sensitivity analyses. The storage coefficient was $2.75x10^{-4}$. One hypothesis to be tested was whether the single field transmissivity determination of 3,500-5,000 ft^2/d in the third strip could represent a limestone aquifer anomaly, and that the true parameter value in this area might be lower, perhaps the same as that of the second strip where better data control was available. The transmissivity value of the third strip was set equal to 1,500 ft^2/d for testing. Computed water levels from the test run and from the control are shown in figures 10 and 12, which also show the observed data. All computed curves for each monitor well start with the same initial water level, but only the last 8 years are illustrated. The computed curves have been shifted by the indicated amounts.

The two monitor wells chosen for the comparison, the south monitor well, injection site 1, in the first strip, and the deep test monitor well, injection site 2, in the second strip, were selected because of the long time span of their water-level records, which included time periods of rising and falling average injection rates. Setting T = 1,500 ft^2/d in the third strip induced "transmissivity buildup" (a cumulative bias) at both wells, so that observed and computed water-level responses no longer agree. The response at regional monitor well 1, where the field determination of transmissivity was made, was also incorrect. Thus, the hypothesis that the third strip transmissivity value should be 1,500 ft^2/d was rejected.

This did not prove that the third strip transmissivity is uniformly 4,000 ft^2/d. Confidence resides in this value only near regional monitor well 1, where water-level data are available. The transmissivity in other parts of the strip might vary considerably. The analysis depended upon the assumption that there is no significant leakage from the injection zone within the model boundaries. If this were not true, the actual transmissivity value might be lower with apparent agreement between computed and measured water levels caused by leakage.

A test run was made with storage coefficient set equal to a value of $2.0x10^{-4}$, lower than that ($2.75x10^{4}$) of the calibrated model used for control, a parameter variation of 37.5 percent. Resulting water levels at the south monitor well and the deep test monitor well are also illustrated in figures 10 and 12. The illustrations show that $S = 2.0x10^{-4}$ induces too strong a response to changes in injection rate at the monitor wells, whether the response be rising or falling water levels. Thus, the hypothesis that $S = 2.0x10^{-4}$ is rejected. Again, confidence resides in the calibrated value of $2.75x10^{-4}$ only at the locations where data are available; in other parts of the modeled region, the true value might vary.

A conclusion of the analyses is that computed water levels are sensitive to moderate variations in both transmissivity and storage parameters. Calibration techniques used in the transient response simulation are illustrated by the sensitivity analyses. The transmissivity error in an extensive distant area (with respect to the two injection site monitor wells) induced a cumulative bias at both wells. The storage coefficient error in both local and distant areas induced a combination of amplitude and bias errors. The initial response to an injection rate change in 1971, when computations incorporate the storage coefficient error, is larger than that due to the transmissivity error. However, in 1974 and later, the water-level deviation caused by the transmissivity error is larger than that caused by the storage coefficient error.

The analyses that were performed are by no means exhaustive of those which might be considered of interest within the context of this study. The use of image well analysis to test the influence of flow system boundaries, described earlier, served a similar purpose. However, the few data control points, scanty data base, and the generalized nature of the regional flow system model limit the need for sensitivity analyses of a high degree of precision.

Predictive Utility of Hydraulic Models

The validation of a model calibration is the establishment of its reliability as a predictive tool. The question to be resolved is whether the model will always predict the correct response (water levels) to varying values of the stress (injection rates) using the parameter values (transmissivity and storage) determined during calibration.

Evidently, increased confidence in the model's predictive ability is acquired if the model is observed to predict correctly for many different levels of the stress. The degree of confidence depends upon the precision of the data, the magnitude of the difference between stress levels, and the number of such distinct stress-level data sets. In this study, many sets of water-level responses from time periods of differing long-term average injection rates were available for calibration, and thus substantial confidence in the model was achieved.

The calibrated model will accurately simulate the water-level response at the various monitor wells where a match was achieved in the calibration process. However, parameters representing hydraulic characteristics of the injection zone were generalized to large parts of the study area on the basis of measurements very distant from some parts of those areas. This meant that the accuracy of the simulation at observation wells did not prove that those parameters were truly representative of parts of the study area lacking data control, but only that the composite effect of the uniform parameter assignment to the larger region "worked" for the restricted part of the area where data control was available. Thus, parameter assignments in areas lacking data control cannot be considered reliable, nor can water-level changes computed for those areas. As new water-level data or new measurements of injection zone aquifer characteristics become available from areas currently without data control, these data should be used to refine the hydraulic calibrations.

Simulating the regional effects of future waste injection at wells other than the ones now operating depends upon their location with respect to the location of existing data, and upon whatever additional hydrogeological information would be made available. If planned well locations are near the sites where information is currently available, such simulations may not require additional calibration. However, if they are in areas currently without data control, little confidence can be attached to simulations unless geohydrologic information from those areas is obtained.

REGIONAL AND LOCAL MOVEMENT OF SALINE NATIVE WATER AND INJECTED WASTEWATER

Interpretation of Hydraulic Models

The following discussion has as its basis the superposition of computed water-level increases upon the model of the regional flow system (figs. 17 and 19). The reader should be aware of previously cited qualifications regarding the regional flow systems illustrated in figures 9, 17, and 19, owing to the scanty areal distribution of data control and the lack of information about some aquifer boundaries. Contours are with respect to sea level and water levels are with respect to a density representing a native water concentration of 5,000 mg/L of dissolved solids.

Both August 1977 water levels (fig. 17) and water levels representing equilibrium at 1978 rates (fig. 19) show a trough northwest of the injection sites where the regional flow gradient balances that from the injection systems. The 1977 map shows this trough to be centered somewhere between the 170-foot contours, with intervening water levels decreasing a few more feet. The equilibrium map (fig. 19) shows the trough to be slightly further northwest between the 210-foot contours, with intervening water levels decreasing several feet more. North and northwest of the trough, southward flow from recharge areas divides to circumvent an area including the injection wells within which the prevailing direction of flow is outward from the injection sites. Within this area surrounding the injection wells, radial, outflow is gradually entrained by the regional flow system with progressive distance from the injection sites until its influence upon the flow direction becomes negligible compared to the regional gradient. Figures 17 and 19 show this to occur well south of the northern and northeastern limit of the Bucatunna Clay, as water-level contours remain approximately normal to this boundary and southeasterly flow prevails as it did before injection (fig. 9). Thus, at 1978 rates, the injection systems should not affect regional flow where the lower limestone of the Floridan aquifer is unconfined to the northeast.

Another flow trough (not illustrated) occurs between the two injection sites where their hydraulic gradients balance. This is closer to injection site 2 because the average injection rate there is considerably lower. Southeastward of the injection sites, the flow direction is similar to that before injection (fig. 9), but flow is more rapid. Virtually all water flowing southeastward from the injection sites is shown to discharge at model boundaries in the Gulf of Mexico, where little is actually known about the extent of the injection zone or confining layer. However, as previously indicated, correct specification of constant-head boundary values at the presumed gulf subcrop, and consideration of declining water levels east of Fort Walton Beach would likely cause a more easterly flow system. A curved streamline can be drawn (fig. 19) from injection site 1 to the vicinity of Fort Walton Beach, where the injection zone is separated from the upper limestone of the Floridan aquifer for about 20 miles further east. This shows that there is a waste flow path to Fort Walton Beach which is, however, hydraulically isolated from Fort Walton Beach pumping wells in the upper Floridan.

Interest has focused upon the extent and direction of the movement of the injected waste and of saline water which resided near the injection sites prior to injection. The actual movement of water impelled by the regional gradient or by gradients from the injection sites is slow at appreciable distances from the injection wells. The regional gradient was shown in simulations to cause flow of 8 to 11 ft/yr at the injection sites, given generalized estimates of aquifer characteristics.

If the volume of injected waste (V) is known at some time (t), as is the thickness of the uniform isotropic receiving zone (b) and the porosity (Θ), then its relation to the radius of the cylindrical waste body (r) is: $V = \pi r^2 b\Theta$, which is equivalent to $r = (V/\pi b\Theta)^{\frac{1}{2}}$. If Q is the current injection rate, the outward speed of interface movement is:

$$\frac{dr}{dt} = \frac{Q}{2(\pi b\theta V)^{\frac{1}{2}}} = \frac{Q}{2\pi r b\theta} \qquad (6)$$

In early 1978, the volume injected at site 1 was about $14.6\text{x}10^9$ gallons, and the current average injection rate was about 2,000 gal/min. Assuming a porosity of 28 percent, and uniform isotropic flow within a 60-foot injection zone, the radius of the cylindrical waste body, disregarding dispersion, would be 6,080 feet (1.15 miles) and the outward movement of this radial limit and adjacent saline water would be at a rate of 219 ft/yr. In early 1978, about $0.89\text{x}10^9$ gal. of waste had been injected at site 2 and the average rate was about 550 gal/min. With the same hydrogeologic assumptions, the radius of the waste body about the American Cyanamid Company primary injection well would be about 1,500 feet (0.28 mile) and the outward speed of the interface would be at a rate of 244 ft/yr. The cylindrical waste slug about the American Cyanamid Company well is much smaller, and therefore expands faster, than the waste about the Monsanto Company wells, even though the injection rate is lower.

However, if outward flow is not uniform within a 60-foot interval of the aquifer, and preferred flow zones exist, the radius of the waste body and its rate of outward movement could be appreciably greater in the preferred flow zones, as would also be the rate of regional flow. If hydraulic properties of the aquifer were anisotropic within the plane of flow, the rate and extent of waste movement would be greater in preferred lateral flow directions. Thus, the estimated radii and outflow rates are conservative in that actual outflow distances and rates might be greater in some sections of the aquifer. Since the estimated values of outflow are large compared to the regional flow rates, the movement of the waste in the vicinity of the wells is approximately radial if the aquifer is isotropic.

Saline water surrounding the expanding body of injected waste will also move radially outward in all directions, including toward the northeast where the aquifer water freshens. The outward flow speed of saline water surrounding injection site 1 would decrease to 50 ft/yr 5 miles from the wells, and to 12 ft/yr 20 miles from the wells, the latter speed comparable with the regional flow movement. If the porosity of the aquifer were half (14 percent) of that assumed in the calculations, the estimated radii of the waste bodies and the outward rates of interface movement would be increased by a factor of 1.414.

To provide perspective concerning the amount of time required for the injected waste, and surrounding saline water driven before it, to move to locations of hydrologic significance in a regional context, three flow paths were considered for approximate travel time calculations (fig. 19). The paths were subdivided, and water particle velocity estimated for each subpath from the local transmissivity and hydraulic gradient. A travel time was obtained from comparing the velocity with the length of the subpath. Hydrogeologic assumptions were the same used in estimating waste movement about the injection wells.

Flow path 1-C′ extends from injection site 1 to the southernmost extent of the Foshee Fault in north central Santa Rosa County, as tentatively indicated by Marsh (1966). The system of faults is known to have affected the Bucatunna confining layer, although it is likely that the degree of faulting is not sufficient to have breached it (Marsh, 1966). The unlikely possibility that waste moving through the aquifer from the injection sites might leak upward near the southernmost extent of the fault where the offset is negligible (point C′) can be considered by water managers as a conservative test of the possibility of upward leakage of waste farther north where the offset is greater.

The flow path is divided into three segments: (1) from the north monitor well near injection site 1, where the equilibrium water level was computed to be 330 feet above sea level, to the 200-foot contour; (2) from the 200-foot contour to the boundary where the transmissivity estimate changes from 850 ft/d to 1,500 ft/d, at which point the water level is estimated to be 170 feet above sea level; and (3) from the preceding point to point C′ which conveniently lies on the 150 foot contour. The three segment lengths are estimated to be about 10.5 miles, 7 miles, and 4 miles. The first two segments lie within the 850 ft/d transmissivity strip, the third lies in the 1,500 ft/d transmissivity strip. As the waste would move much more rapidly in the interval between the injection well and the north monitor well, this segment is neglected. Average flow speeds (v) in the path segments are estimated as $v = \frac{T}{\theta b}\frac{\Delta h}{\Delta \ell}$, where T is transmissivity (L/T), θ is porosity, b is layer thickness (L), Δh is the head loss (L) on the path segment of length $\Delta \ell$ (L). Estimated fluid particle speeds for the three path segments are 43.3, 15.0, and 30.9 ft/yr. Then the total estimated traveltime is:

$$\sum_{i=1}^{3} \frac{\Delta \ell_i}{v_i} = \left\{ \frac{10.5 \text{ mi}}{43.3 \text{ ft/yr}} + \frac{7 \text{ mi}}{15 \text{ ft/yr}} + \frac{4 \text{ mi}}{30.9 \text{ ft/yr}} \right\} \times \frac{5{,}280 \text{ ft}}{1 \text{ mi}} = 4{,}429 \text{ yr}$$

Thus, based upon the simulated equilibrium water levels (fig. 19), more than 4,000 years would be required for injected waste to move to point C′.

In northern Escambia and Santa Rosa Counties, the injection zone native water chloride concentration is below or near the maximum (250 mg/L) usually deemed acceptable for public consumption. Most flow of saline water from the vicinity of the injection systems is deflected from northern Escambia County by the regional flow system, but with sufficient time could enter parts of northern Santa Rosa County. Point C′ in this area is useful for assessing the likelihood that saline water driven from the injection sites could affect a well used for water supply. The flow path through point C′ (fig. 19) originating at injection site 1 likely passes entirely through a region where water is more saline that at point C′, if the hypothesis of a freshwater interface with saline water to the southwest holds true. Near point C′, the flow path is oblique to the presumed southwest direction of the chloride gradient. From a consideration of the local equilibrium water levels (fig. 19), the rate of water movement in the aquifer would be between 25 and 30 ft/yr. It would take from 170 to 210 years for water to move 1 mile downgradient. As water 1 mile upgradient would likely not be appreciably more saline, little change in chloride concentration would occur at a local well in that time period.

Flow path 1-C′′ extends from injection site 1 to regional monitor well 2, where the chloride concentration (400 mg/L) was not much higher than the potability limit. Flow path 1-C′′ is appreciably shorter than 1-C′, but injected waste and associated saline water would still require over 1,800 years to traverse the distance, based upon a travel time computation in which the flow path is divided into two 8-mile segments at the boundary between transmissivity strips where the flow path also intersects the 200-foot contour. End point water levels are estimated as 330 feet above sea level (north monitor well) and 150 feet above sea level at point C′′.

Flow path 1-C′′′ extends obliquely from injection site 1 to Fort Walton Beach, where the upper Floridan is the primary source of water supply. The intervening Bucatunna, estimated to extend eastward for another 20 miles, protects the source of public supply from contamination by water from the saline lower Floridan, yet it may be of interest that the estimated time of travel from the injection site to the Fort Walton Beach area is over 5,800 years, from a similar analysis dividing the flow path into six segments at the boundaries between transmissivity strips (water levels estimated to be 250 feet and 130 feet above sea level) and at the 200-, 150-, and 100-foot contours. Flow path and endpoint water levels were 330 feet (north monitor well) and 55 feet above sea level at Fort Walton Beach.

If porosity in the aquifer were half (14 percent) of that assumed in the analyses, the speed of movement of water along the flow paths would be doubled and the computed traveltimes halved. The travel time estimates are based upon broad generalizations concerning the hydraulic characteristics of the injection zone and upon unproven assumptions of uniform, isotropic flow in a 60-foot interval, and must be carefully qualified. However, they serve to illustrate that the amount of time required for injected waste and surrounding native saline water to move an appreciable distance from the injection sites is probably orders of magnitude greater than the probable lifetime of the present underground waste disposal operations in northwestern Florida.

Modeling the Transport of Injected Waste

Approach

Ideally, it would have been advantageous to follow the two-dimensional flow model calibration with a multilayered hydraulic simulation using SWIP into which a simulation of the transport of the waste fluid could be incorporated. The additional hydraulic data required by SWIP for transport computations (the thickness, porosity, and permeability of distinct intervals within the receiving zone) would be estimated from an interpretation of flow meter surveys, geophysical logs, and time series of chemical data measured at various observation wells. This is because the outward movement, in contrasting layers, of the interface between injected and resident fluids depends upon the relative permeability, thickness, and porosity of the layers. Incorporation of the waste transport calculations would also motivate use of the chemical data to estimate hydrodynamic dispersion, the mixing of injected and native waters about their common interface. If chemical data were available only from one observation well, use of the data for these purposes would require the assumption that flow in the aquifer was approximately uniform and isotropic. If several or many wells provided data, this assumption could either be confirmed by the data, or anisotropy could be simulated by the model.

The hydraulic conductivity of the injection zone was known to be vertically heterogeneous. However, the flow meter data were insufficient for local differentiation of layers on the basis of hydraulic properties. No basis existed for the hydraulic differentiation of layers on an areal basis, and the construction of a multilayered model for solute transport simulation was not possible. The amount and distribution of chemical data showing the arrival of waste was insufficient to determine the degree of anisotropy. A simplifying assumption of vertical hydraulic uniformity and isotropic flow in the most-permeable part of the injection zone had to be made, and transport calculations were incorporated into the single layer flow simulation with SWIP described in preceding sections.

Incorporating a simulation of waste transport required some estimate to be made of the degree of hydrodynamic dispersion, which is represented in most transport models by the specification of the dispersivity parameter (α). Considered a "characteristic length," it is expressed in length units (feet). The dispersion coefficient (E) is then computed as the product of the dispersivity parameter and the speed of flow (u) in velocity units (ft/d). SWIP uses two dispersivity parameters, longitudinal (α_ℓ) and transverse (α_t) dispersivities. The first specifies the degree of dispersion in the direction of flow, the second the degree of dispersion in the plane perpendicular to the direction of flow.

Ehrlich and others (1979) estimated a longitudinal dispersivity parameter of approximately 30 feet, based upon the amount of time required for a fairly stable concentration of thiocyanate (SCN) injected at the American Cyanamid Company primary injection well to arrive at the deep test monitor well, and upon the estimated thickness (60 feet) and effective porosity (28 percent) of the zone through which the waste moved. These same hydrogeologic parameters were used for an estimate of the time of arrival of hypothetical plug flow at the deep test monitor well, and it was found that this time corresponded closely to the actual time of arrival of an SCN concentration of 50 percent of the average injected concentration. (Plug flow means that the injected fluid forms an enlarging cylinder without any dispersion at its boundary, and its radius is considered to correspond approximately to the 50 percent injected (or native) water concentration at the centroid of a mirror-symmetrical transition zone between the waters which is caused by dispersion.) This calculation tended to confirm the estimate of the hydrogeologic parameters used in the dispersivity calculation, given the assumption of uniform, isotropic radial flow from the injection well.

The dispersivity parameter estimate of Ehrlich and others (1979) was based upon a technique which considers only dispersion in the direction of flow, so their value of 30 feet was entered into SWIP as the value of longitudinal dispersivity. As SWIP also simulates transverse dispersion, a transverse dispersivity parameter needed to be estimated. Transverse dispersion is usually regarded as being of lesser degree than longitudinal dispersion (Faust and Mercer, 1980), so a value of 10 feet was arbitrarily chosen. Both coefficients were considered to be uniform within the entire modeled area. Neither confirmation nor refutation of these parameter choices was achieved by model simulation.

Resulting Numerical Problems

In order to determine which finite differencing method would provide a numerically stable and accurate computation of the waste fluid distribution, several were tried. The centered-in-time and centered-in-space (Crank-Nicholson) method was found to produce large oscillations at the interface between injected and native waters in successive time steps. Since SWIP limits the interval between time steps on the basis of the concentration change at grid nodes, these large oscillations meant that a very large number of time steps were required to simulate a short time period, and large computer costs were incurred while producing a simulation of limited usefulness. Numerical criteria are presented in the documentation by INTERCOMP Resource Development and Engineering, Inc. (1976) which would mitigate these oscillations. To satisfy these criteria, substantially smaller grid cells and time steps would be required, which would have been infeasible in view of the large time and spatial scale of the problem.

A backward-in-time (implicit) method was also tested, together with a centered-in-space approach to the spatial derivatives in the convective terms. Some numerical dispersion was introduced into the solution by the backward-in-time difference, and some oscillation was introduced by the centered-in-space difference. These latter oscillations were found, however, to be far smaller in magnitude than the ones generated by the centered-in-time difference. They were most noticeable near the injection well grid nodes, where conceptually meaningless solute fraction values as large as 1.06 were computed. The degree of numerical dispersion was major, however, and efforts were made to assess its significance.

Numerical dispersion (from the backward-in-time difference), indistinguishable in computations from the simulation of physical dispersion, is related to the speed of outward movement of the waste front (u) and to the computational time step (Δt) according to the relation $u^2\Delta t/2\Phi$, where Φ is the effective porosity (INTERCOMP, 1976). The formula for numerical dispersion and the expression for dispersion in the direction of flow ($\alpha_\ell u$) both depend upon the flow velocity (u), which can be divided out of the numerical dispersion formula to produce the expression $u\Delta t/2\Phi$, herewith termed "time-wise numerical dispersivity," in length units (feet). Depending upon flow velocity and time step size, it can be used for a direct quantitative comparison with the dispersivity parameter (α_ℓ) specifying the degree of physical dispersion.

Estimates were made of time-wise numerical dispersivity during the 15-year time period of the simulation. In grid blocks corresponding to locations of the waste front movement from injection site 1 in the first few days of the simulation, time-wise numerical dispersivity was of the order of 25 to 50 feet for time steps of 2 to 3 days. This high value was due to the high outward speed of expansion of the small cylindrical injected waste body. After 3,000 days of injection, when the outward speed of the waste front had decreased to 0.9 to 1.1 ft/d, time-wise numerical dispersivity ranged from 35 feet for an 18-day time step to 532 feet for a 335-day time step. After 5,175 days (August 1977) the estimate was 256 feet for a 203-day time step.

These values are very large compared to the estimated physical dispersivity (α_ℓ) of 30 feet, indicating that the apparent dispersion introduced by the backward-in-time difference method and the time step sizes dominated the hydrodynamic dispersion thought actually to occur. This should lead in theory to a degree of "smearing" of the simulated interface between injected wastewater and native water substantially greater than that actually observed. Smaller time steps could have been used, but the number required to simulate 15 years of injection would have been uneconomical.

Other numerical methods did not provide better results. A disadvantage of using the backward-in-space method was that it tended to increase the level of numerical dispersion. The degree of numerical dispersion inherent in the backward-in-time, backward-in-space difference option is the sum of the previously computed estimate $u^2\Delta t/2\Phi$, plus an additional term related to the size of the grid block, $u\Delta x/2$. The mathematical expression for the numerical dispersion introduced by the backward-in-space difference ($u\Delta x/2$) is divided by the velocity (u) to produce a quantity herewith termed "spatial numerical dispersivity." In length units and simply equal to half the grid block dimension, it is directly comparable to the longitudinal dispersivity parameter (α_ℓ). The magnitude of spatial numerical dispersivity in the SWIP run ranged from 100 feet to 1,500 feet, very large compared to the degree of physical dispersion. Again, this would in theory cause a major increase in apparent simulated dispersion over that intended by the specification of 30 feet for longitudinal dispersivity (α_ℓ). Smaller grid cells could have been used, but the large size of the solution matrix would have been uneconomical for computer processing.

The computed solution for waste front movement using the backward-in-time, centered-in-space difference did not agree with observed data. The SWIP simulation did not predict the arrival of waste at the south monitor well at injection site 1 until 1980, although it is known to have actually been detected there in 1974 (Pascale and Martin, 1978). The simulation showed too early an arrival of waste fluid at the deep test monitor well and standby injection well at injection site 2, followed by too attenuated a rate of injected fluid concentration increase. The simulated time of arrival at the deep test monitor well of the 50 percent waste fluid concentration was much later than the one described by Ehrlich and others (1979). It was 40 percent later (205 days) than the calculated arrival of hypothetical plug flow.

Lack of agreement between model computations and observed chemical data would have occurred if model assumptions of uniform isotropic flow within a vertically homogeneous aquifer were sufficiently unrepresentative of the injection zone near the injection wells. However, the plug flow radius should have been consistent with the simulated 50 percent concentration arrival time, as both estimates are based upon those assumptions. A moderate error in the dispersivity parameter value would have tended to widen or narrow the transition zone, while leaving the centroid (50 percent concentration radius) relatively unchanged. The large increase in apparent dispersion introduced by the backward differencing technique would be expected to produce the same effect to a greater degree. It is not known whether the high degree of numerical dispersion could have distorted the transition zone to the extent that its centroid no longer corresponded to the 50 percent concentration radius. Allowing for the possibilities of incorrect model setup or interpretation of results, or an error in the 1977 version of the SWIP code, resolution of this problem awaits further study.

Despite computational problems, a roughly circular waste fluid body was portrayed by the simulation, depicting approximately radial flow of the waste governed by hydraulic gradients from the well. Greater success might have been achieved with small-scale simulations of the waste transport about the injection wells than with the large-scale approach of this study. Additional data describing the vertical distribution of flow and hydraulic characteristics, dispersion, and anisotropy would enhance the value of such small-scale simulations.

SUMMARY

The hydraulic effects of waste injection at two sites in northwest Florida were simulated with digital models to provide concerned agencies with a regional portrayal of changing water levels, and to demonstrate the capabilities of models available for such simulations. A two-dimensional flow model was considered appropriate for simulation of the prevailing flow and boundary conditions. Steady-state simulations were made to enhance understanding the natural, prestress regional flow system and its effect upon the movement of the waste. Transient (time-varying) simulations, matching the observed water-level changes at monitor wells, portrayed the regional hydraulic effects of injection.

A very large grid was designed for a preliminary model which represented an effectively unbounded aquifer. This assured that appreciable water-level changes would not occur near the locations of simulation boundaries even after 15 years of injection, and permitted the specification of constant head conditions at those boundaries. Transmissivity values of 850, 1,500, and 4,000 ft^2/d were assigned to three vertical strips. A storage coefficient value of 2.75×10^{-4} was selected for the entire modeled area on the basis of calibration runs. The calibrated model provided a satisfactory match between computed and observed water levels at monitor wells near the injection sites. At the more distant regional monitor wells, the slopes of the computed response curves deviated from the observed ones. Image wells were located to the northeast to represent the influence of the northeastern pinchout of the confining layer. The revised computed response curves at the regional monitor wells then matched the observed ones.

Natural aquifer boundaries were incorporated into the model. Estimates of water levels at constant head boundaries were based upon values acquired in the course of previous areal studies in Florida and Alabama. The resultant pattern of prestress, steady-state water-level contours was similar to that of the data-based contours, and supported the interpretation of a south-easterly flow regime. The transient hydraulic response of the aquifer to injection was recomputed. Water-level response curves were similar to those computed when the northeastern boundary was represented by an image well, and agreed well with observed data. A computed cumulative water budget for August 1977 showed that 1.95×10^9 ft^3 of water had been injected, and that 1.29×10^9 ft^3 of additional storage in the aquifer had been created by the high pressures caused by injection.

Steady-state and transient simulations computed using the subsurface waste disposal model (SWIP) were very similar to those computed by the two-dimensional flow model. It was found that a porosity value of 28 percent, a permeable zone depth of 59.5 feet, and a value of 3.5×10^{-5} in^2/lb for the compressibility of the aquifer material were equivalent to the storage coefficient of 2.75×10^{-4} used in the two-dimensional flow model and were consistent with various field measurements. The equilibrium water-level response of the injection zone to the continuation of injection at 1978 rates was simulated, and water levels were not substantially greater than computed 1978 water levels, indicating that the aquifer was approaching steady-state with respect to these rates in 1978.

The regional flow system influenced by the waste injection systems has a water-level trough northwest of the injection sites where regional flow divides to circumvent an area containing the sites. Within this area flow is outward from the injection wells until, with progressive distance from the wells, it is entrained by regional flow. The northeast limit of the Bucatunna confining layer is sufficiently distant for the natural flow gradient there to be virtually unaffected by injection. Simulated regional flow patterns near the eastern, southeastern, and southern (subcrop) boundaries are probably inaccurate because: (1) constant-head value specifications along the subcrop boundary were too low; (2) some degree of confinement might occur, contrary to model assumptions, to the east of the eastern pinchout of the Bucatunna; and (3) appreciable drawdowns from heavy pumping near Fort Walton Beach during the time period of the simulation influenced injection zone water levels along the eastern model boundary but were not simulated.

Estimates were made of the traveltime between injection site 1 and three points of regional hydrologic significance. If the flow zone were uniform, isotropic, and 60 feet thick with 28 percent porosity, it would take over 4,400 years for injected waste to reach the nearest part of the Foshee Fault, where aquifer water is potable, and over 1,800 years to reach regional monitor well 2, where aquifer water is only slightly brackish. At a sample point in northern Santa Rosa County, the flow speed was estimated to be from 25 to 30 ft/yr, suggesting that, on a regional basis, the northward movement of saltwater would not affect freshwater supply for many hundreds of years. The curved flow path to Fort Walton Beach had a traveltime of over 5,800 years. The estimated traveltimes would be less if flow were in discrete zones within the 60-foot interval, were anisotropic, or if the porosity were much less than 28 percent.

As to the significance of the investigation, not all of the anticipated results of the investigation were fully achieved, but worthwhile products emerged from the principal lines of endeavor, which were: (1) simulation of the regional flow system; (2) simulation of observed injection-zone water-level changes at various observation wells; and (3) incorporation of a waste transport simulation into a regional hydraulic model. The first line of endeavor led to a highly generalized regional flow model based upon a few known and reconstructed water levels and upon limited evidence describing aquifer water quality and flow system boundaries. The second line of endeavor fully achieved its objective. A two-dimensional flow model was found to be quite suitable for both analyses. Together, the results made possible highly generalized portrayals of historical and future changes in the regional flow system caused by the waste injection operations. The indicated changes were used for general interpretations concerning the local and regional movement of injected waste and native saline waters.

The third line of endeavor entailed the transfer of the flow solution to the SWIP model to provide the framework for a transport simulation. However, it was found that, in the transport calculations, numerical problems occurred which could not be overcome within the limited budget and time frame of the study, although the flow solution was successfully replicated. The product of this line of endeavor is understood to be insight gained into the effect of time step and grid size constraints (to mitigate numerical problems) upon the feasibility of applying a finite-difference model (SWIP) to a field problem of solute transport.

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