Simulation of Subsurface Storage and Recovery of Treated Effluent Injected in a Saline Aquifer, St. Petersburg, Florida

By Dann K. Yobbi

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CONTENTS

FIGURES

TABLES

CONVERSION FACTORS, VERTICAL DATUM, ABBREVIATIONS, AND ACRONYMS

Multiply inch-pound unit	By	To obtain
foot (ft)	0.3048	meter
mile (mi)	1.609	kilometer
foot squared (ft^2)	0.0929	meter squared
foot per day (ft/d)	0.3048	meter per day
foot squared per day (ft^2/d)	0.0920	square meter
foot squared per pound (ft^2/lb)	$1.007x10^{-6}$	square meter per Newton
inch squared per day (in^2/lb)	$1.45x10^{-4}$	square meter per Newton
pounds per square inch (lb/in^2)	6.895	kilopascal
pounds per cubic foot (lb/ft^3)	0.0160	gram per cubic centmeter
million gallons per day (Mgal/d)	0.4381	cubic meter per second

Equation for temperature conversion between degrees Celsius (oC) and degrees Fahrenheit (oF):

$$^oC = 5/9 \text{ x } (^oF-32)$$
$$^oF = (9/5\ ^oC) + 32$$

Sea level: In this report, “sea level” refers to the National Geodetic Vertical Datum of 1929 (NGVD of 1929)---a geodetic datum derived from a general adjustment of the first-order level nets of the United States and Canada, formerly called “Sea Level Datum of 1929.”

ADDITIONAL ABBREVIATIONS

mg/L	milligrams per liter
α_T	transverse dispersivity
α_L	longitudinal dispersivity
k_h	horizontal permeability
k_v	vertical permeability

ACRONYMS:

AIF	aquifer influence function
DS	dissolved solids
HST3D	U.S. Geological Survey Three Dimensional Heat- and Solute-Transport computer program
PHREEQE	U.S. Geological Survey equilibrium speciation computer program for geochemical calculations
SSMF	scaled-solute mass fraction
SSR	subsurface storage and recovery
SWFWMD	Southwest Florida Water Management District
SI	saturation index
USGS	U.S. Geological Survey
WATEQF	U.S. Geological Survey equilibrium speciation computer program for natural waters
WRF	water reclamation facilities

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Abstract

The potential for subsurface storage and recovery of treated effluent into the uppermost producing zone (zone A) of the Upper Floridan aquifer in St. Petersburg, Florida, is being studied by the U.S. Geological Survey, in cooperation with the city of St. Petersburg and the Southwest Florida Water Management District. A measure of the success of this practice is the recovery efficiency, or the quantity of water relative to the quantity injected, that can be recovered before the water that is withdrawn fails to meet water-quality standards. The feasibility of this practice will depend upon the ability of the injected zone to receive, store, and discharge the injected fluid.

A cylindrical model of ground-water flow and solute transport, incorporating available data on aquifer properties and water quality, was developed to determine the relation of recovery efficiency to various aquifer and fluid properties that could prevail in the study area. The reference case for testing was a base model considered representative of the saline aquifer underlying St. Petersburg. Parameter variations in the tests represent possible variations in aquifer conditions in the area. The model also was used to study the effect of various cyclic injection and withdrawal schemes on the recovery efficiency of the well and aquifer system.

A base simulation assuming 15 days of injection of effluent at a rate of 1.0 million gallons per day and 15 days of withdrawal at a rate of 1.0 million gallons per day was used as reference to compare changes in various hydraulic and chemical parameters on recovery efficiency. A recovery efficiency of 20 percent was estimated for the base simulation. For practical ranges of hydraulic and fluid properties that could prevail in the study area, the model analysis indicates that (1) the greater the density contrast between injected and resident formation water, the lower the recovery efficiency, (2) recovery efficiency decreases significantly as dispersion increases, (3) high formation permeability favors low recovery efficiencies, and (4) porosity and anisotropy have little effect on recovery efficiencies. In several hypothetical tests, the recovery efficiency fluctuated between about 4 and 76 percent.

The sensitivity of recovery efficiency to variations in the rate and duration of injection (0.25, 0.50, 1.0, and 2.0 million gallons per day) and withdrawal cycles (60, 180, and 365 days) was determined. For a given operational scheme, recovery efficiency increased as the injection and withdrawal rate is increased. Model results indicate that recovery efficiencies of between about 23 and 37 percent can be obtained for different subsurface storage and recovery schemes. Five successive injection, storage, and recovery cycles can increase the recovery efficiency to about 46 to 62 pecent. There is a larger rate of increase at smaller rates than at larger rates. Over the range of variables studied, recovery efficiency improved with successive cycles, increasing rapidly during initial cycles then more slowly at later cycles.

The operation of a single well used for subsurface storage and recovery appears to be technically feasible under moderately favorable conditions; however, the recovery efficiency is highly dependent upon local physical and operational parameters. A combination of hydraulic, chemical, and operational parameters that minimize dispersion and buoyancy flow, maximizes recovery efficiency. Recovery efficiency was optimal where resident formation water density and permeabilities were relatively similar and low.

INTRODUCTION

The city of St. Petersburg owns and operates one of the largest urban reclaimed-wastewater reuse systems in the world. Currently (1995), approximately 21 Mgal/d of advanced secondary-treated effluent is piped from the city's four water reclamation facilities (WRF) through a 260-mile irrigation system to water residential and commercial properties. Demand for reclaimed water is seasonal. There is a deficiency of effluent for irrigation in the dry months and an excess in the wet months, during which the excess is disposed of through deep underground injection wells. The injected water from these deep permeable zones cannot be effectively recovered because the disposal zone is in a highly fractured dolomite saturated with saltwater (Hickey and Ehrlich, 1984). One solution, known as subsurface storage and recovery (SSR), to this dilemma involves the injection of effluent into shallow, less transmissive formations of low or moderate salinity, by one or more wells, for storage during wet periods when demand is low. The injected water would be withdrawn later for irrgation use during dry periods when demand is high. SSR is especially appropriate for areas like St. Petersburg where there is: (1) seasonal variations in water supply and demand, and (2) availability of moderately permeable aquifers near the surface that contain brackish water.

The feasibility of a SSR system will depend upon the ability of the injected zone to receive, store, and discharge the injected effluent. A measure of the success of a SSR system is the quantity of water that can be recovered relative to the quantity injected, or recovery efficiency. Recovery efficiency, usually expressed as a percentage per cycle of injection, storage, and recovery, is defined as the volume of water recovered before the withdrawn water fails to meet some prescribed chemical standard. In this report, the standard has been taken to be when the water that is withdrawn exceeds a dissolved solids (DS) concentration of 1,500 mg/L.

Two primary physical processes limit the recoverability of the injected water: (1) mixing by advection and hydrodynamic dispersion, and (2) density stratification. Mixing and dispersion creates a diffused zone between the injected and formation waters as a result of molecular diffusion and mechanical dispersion. Density stratification describes the tendency for the lighter fluid to rise above the denser fluid. Unfavorable physical and solute properties of the aquifer system can strengthen these deleterious processes and reduce the recoverability of injected water.

An assessment of the potential recovey efficiency for the aquifer system underlying St. Petersburg needs to be made before a commitment of resources is made for operational testing at a specific site. This requires a semi-quantitative understanding of the dependence of recovery efficiencies on hydrogeologic and chemical characteristics of the aquifer system and on system designs and management parameters. A cost-effective alternative to field testing is simulation modeling, in which many combinations of conditions can be investigated with relatively inexpensive computer simulations.

In 1994, the U.S. Geological Survey (USGS), in cooperation with the city of St. Petersburg and the Southwest Florida Water Management District (SWFWMD), began a model-based investigation of the hydrogeologic and operational aspects of subsurface injection and storage of effluent, and possible future retrieval for nonpotable use. The study area is the city of St. Petersburg, located on the southern tip of Pinellas County (fig. 1).

Throughout this report, statements are made concerning the salinity of water. The terminology used to describe the salinity is modified slightly from a USGS classification system of water based on dissolved solids (Heath, 1989, table 2, p. 65), as follows:

Classification	Dissolved-solids concentration (milligrams per liter)	Percent seawater
Freshwater	<500	<1.5
Slightly saline (brackish water)	500 to 3,000	1.5 to 8.6
Moderately saline (brackish water)	3,000 to 10,000	8.6 to 29
Very saline (saltwater)	10,000 to 35,000	29 to 100
Brine	>35,000	>100

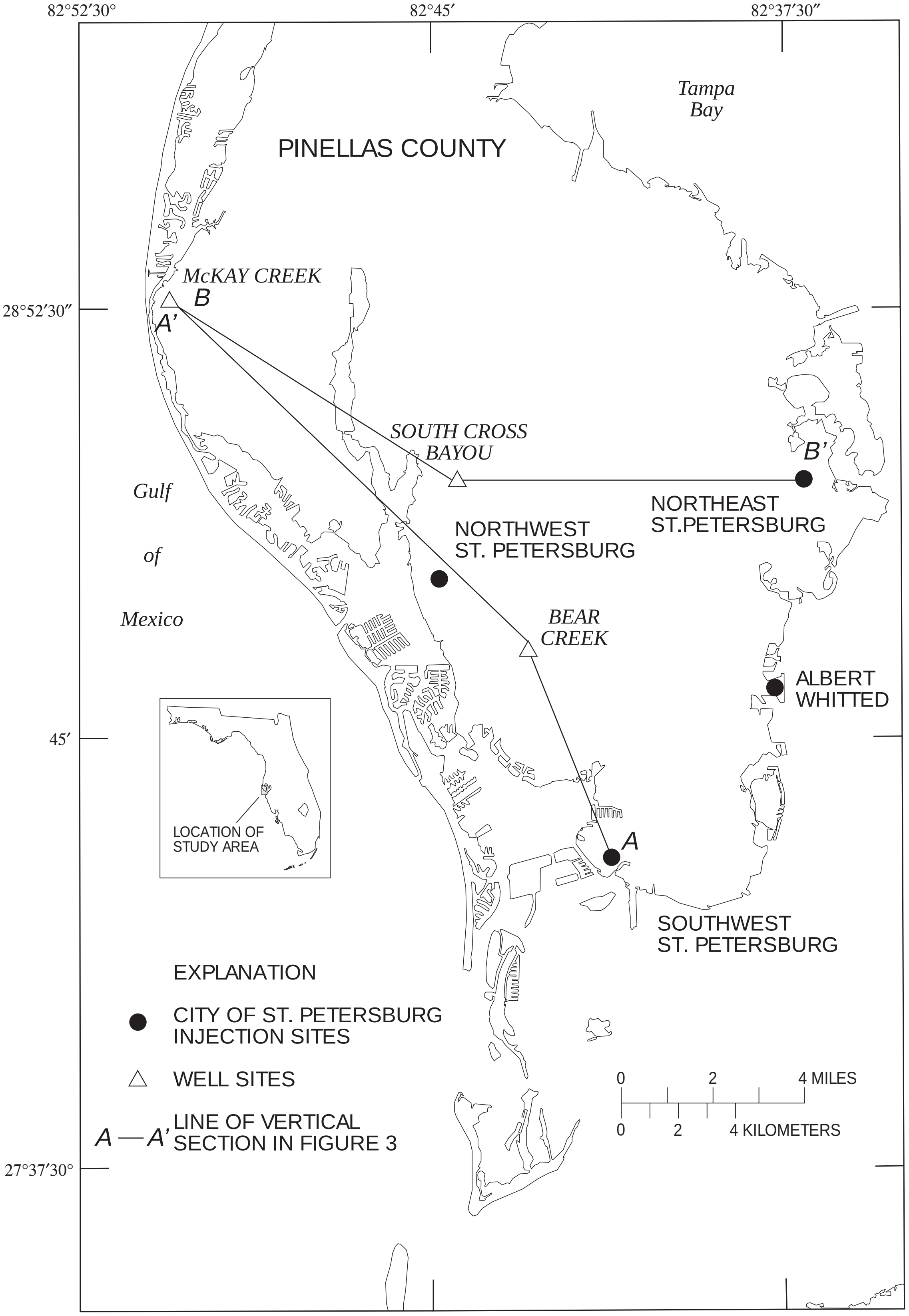


Figure 1. Location of study area, injection sites, and lines of vertical sections.

Freshwater meets the DS concentration limit for potable water. Slightly saline water is nonpotable, but it may be suitable for irrigation. Moderately saline water is suitable for desalinization, and very saline water and brine are considered unusable.

Purpose and Scope

This report presents the results of a study conducted to provide a better understanding of the potential for SSR in a moderately transmissive, slightly to moderately saline-water bearing, limestone aquifer underlying St. Petersburg. Specifically, the objectives are (1) define the hydrogeologic framework and quality of ground water, (2) determine the geochemical interactions associated with SSR, and (3) illustrate the application of a solute-transport model as a tool for understanding the relative importance of individual physical properties and operational variables on recovery efficiency. The scope of the study is limited to a preliminary analysis because no data exist for comparison with model results.

Information on the hydrogeologic framework, hydrologic properties, matrix properties, and water chemistry of the aquifer system was compiled from files of the USGS and from engineering reports of the city’s four WRF injection well sites.

The possibilities for geochemical interactions between the injected and aquifer waters were evaluated using aqueous speciation (WATEQF) and chemical mass-balance (PHREEQE) models (Plummer and others, 1976; Parkhurst and others, 1980). The models were used to assess the potential for both precipitation and dissolution of certain carbonate minerals.

The three dimensional heat-and solute-transport model (HST3D), developed by Kipp (1987), was used to simulate a typical injection/recovery well system. Injection and withdrawal in a prototype aquifer were simulated and recovery efficiency was computed. The model was used to assess the relation of recovery efficiency to various aquifer and fluid properties and to simulate recovery efficiencies under selected hypothetical operational schemes.

HYDROGEOLOGIC FRAMEWORK

The hydrogeologic units beneath the study area consist of a thick sequence of carbonate rock overlain by clastic deposits. The sediments are subdivided into a sequence of discrete lithologic units that form a layered sequence of two aquifers and one confining unit. The framework includes the unconfined, surficial aquifer and the confined, Floridan aquifer system (fig. 2). The units are separated by the intermediate confining unit.

Surficial Aquifer

The surficial aquifer is the uppermost water bearing formation. It consists of undifferentiated sands and clays that vary in composition both laterally and vertically. The aquifer is a source of recharge to the Floridan aquifer system and is mainly used as a source of water for lawn irrigation. The surficial aquifer is generally less than 30 ft thick and is generally saturated to within 10 ft of land surface during dry weather. During wet weather, the water table in the surficial aquifer is generally close to land surface. The surficial aquifer has a horizontal hydraulic conductivity ranging from 13 to 33 ft/d and a vertical hydraulic conductivity ranging from 0.3 to 13 ft/d (Cherry and Brown; 1974; Sinclair, 1974; Hutchinson and Stewart, 1978).

Intermediate Confining Unit

The intermediate confining unit of low-permeability lies between the surficial aquifer and the Floridan aquifer system. The unit coincides with the undifferentiated Arcadia Formation of the Hawthorn Group and consists of a clastic and carbonate sequence. The carbonates in the sequence are generally underlain and overlained by clays and marls of relatively low permeability (Hickey, 1981). Thickness of the intermediate confining unit averages about 90 ft and ranges from about 50 to 140 ft. The confining unit is highly variable both spatially and vertically. A wide range of hydraulic characteristics occurs within the unit due to lithologic heterogeneity within the unit. Vertical hydraulic conductivity for the intermediate confining unit as reported by Sinclair (1974) and Black, Crow, and Eidsness, Inc. (1978) ranges from 1.3×10^{-4} to 6.9×10^{-3} ft/d.

Floridan Aquifer System

The Floridan aquifer system is a thick, regionally extensive sequence of Tertiary age carbonates. Miller (1986) defines the Floridan aquifer system to include the Upper Floridan aquifer, the middle confining unit, and the Lower Floridan aquifer. In the study area, the

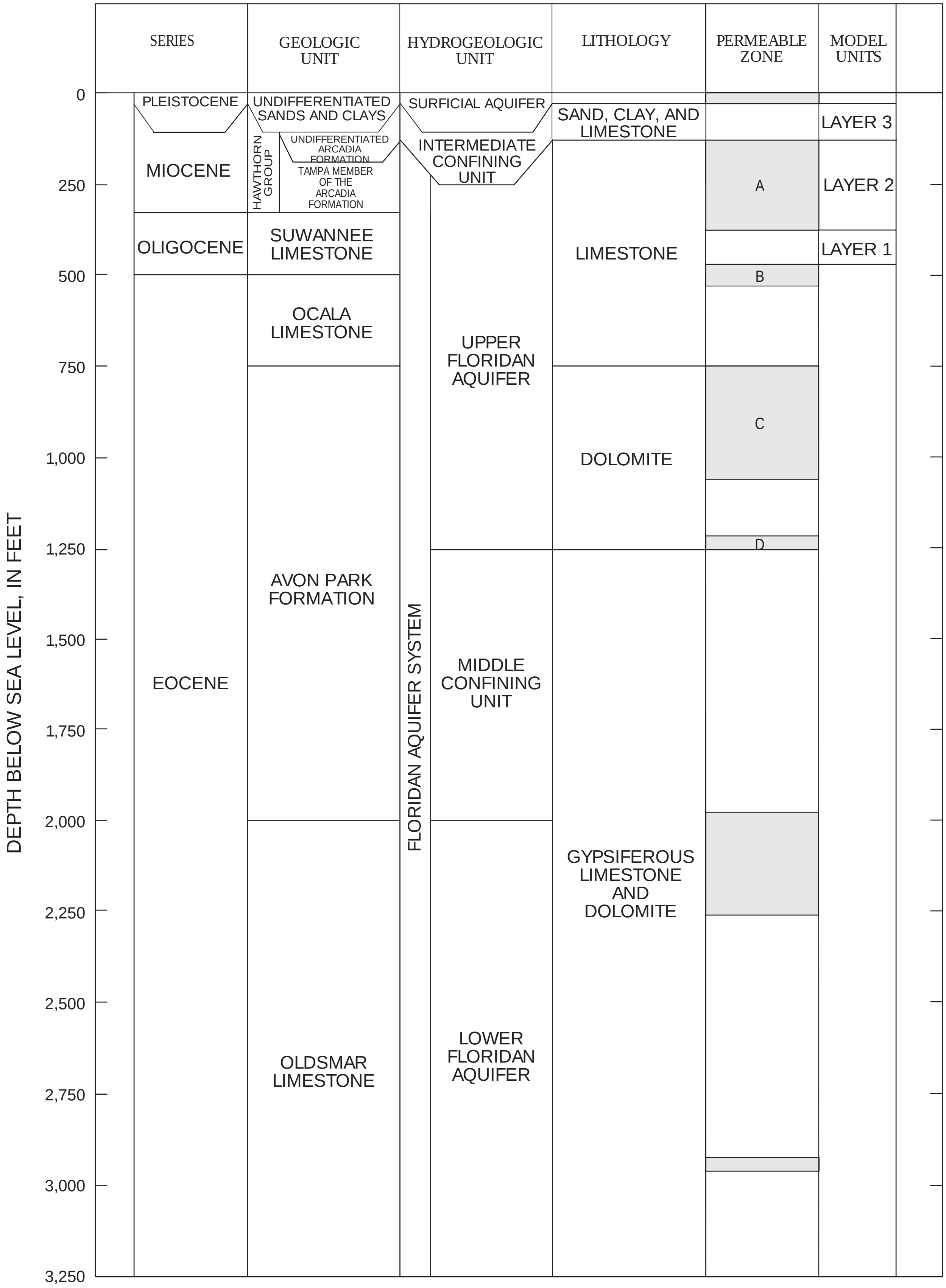


Figure 2. Generalized stratigraphic and hydrogeologic section, Pinellas County. (Modified from Hickey, 1982.)

middle confining unit and the Lower Floridan aquifer contain water comparable to seawater; the base of the freshwater flow system is limited to the Upper Floridan aquifer. The geologic formations that make up the Upper Floridan aquifer consists of limestone and dolomite rocks of, in ascending order, the Avon Park Formation, the Ocala and Suwannee Limestones, and the Tampa Member of the Arcadia Formation of the Hawthorn Group. The top of the Upper Floridan aquifer is defined as the first occurrence of a persistent carbonate sequence; the base of the Upper Floridan aquifer is defined as the first occurrence of interbedded gypsum in the carbonates below a dark-brown, microcrystalline dolomite in the Avon Park Formation (Hickey, 1982). In St. Petersburg, the Upper Floridan aquifer is subdivided into four permeable zones separated by semiconfining units (Hickey, 1982). The zones are alphabetically labeled with increasing depth from A to D (fig. 2). This study is concerned only with the uppermost producing zone of the Upper Floridan aquifer (zone A) , the overlying confining unit, and the underlying semiconfining unit between zone A and B, and further discussion will be restricted to these units.

Zone A

Zone A comprises the Tampa Member of the Arcadia Formation of the Hawthorn Group and the uppermost part of the Suwannee Limestone. Zone A is the shallowest and freshest of the producing zones and is the only potential receiving zone for SSR in St. Petersburg. Thickness of zone A averages about 180 ft and ranges from about 115 to 245 ft. Thickness varies from site to site, occurring with no regional pattern (Hickey, 1982). Geraghty and Miller, Inc. (1976), Robertson and Mallory (1977), Black, Crow, and Eidsness, Inc. (1978), Hickey (1982), and Brown and Associates (1986) reported values of transmissivity for zone A that ranged from 2.2×10^4 to 3.5×10^4 ft^2/d and values of storativity that range from 4×10^{-4} to 8×10^{-4}. Average values of porosity of zone A , estimated from geophysical logs, are 26, 32, and 41 percent (Hickey, 1982).

Semiconfining Unit Between Zones A and B

Underlying zone A (the uppermost permeable zone) is the first of a series of poorly transmissive carbonate rock that acts as semiconfining units that separate permeable zones. The existence of the semiconfining units was determined during previous studies by Hickey (1982). The semiconfining unit below zone A is in the limestone unit of the Suwannee Limestone. Thickness of the semiconfining unit averages about 150 ft and ranges from about 125 to about 170 ft. Average porosity of the semiconfining unit from geophysical logs is about 30 percent and ranges from 22 to 36 percent (Hickey, 1982). The semiconfining unit is considered a nonproducing zone in St. Petersburg.

Vertical hydraulic conductivity of the semiconfining unit between zones A and B, determined from laboratory and aquifer tests reported by Hickey (1982), ranges from 1.3×10^{-3} to 2.6 ft/d. The value of 1.3×10^{-3} ft/d was determined from a laboratory test of a limestone core from the northeast St. Petersburg WRF where a higher percentage of clay occurred in the limestone matrix than at other sites in St. Petersburg. Test results at southwest St. Petersburg WRF and South Cross Bayou indicate that a value of less than 0.1 ft/d probably is not representative of general conditions (Hickey, 1982). Comparison of aquifer and laboratory tests indicate that the plausible range of vertical hydraulic conductivity applicable to semiconfining units that do not contain clay would be in the range of 0.1 to 1.0 ft/d (Hickey, 1982). For the semiconfining beds that contain clay between zones A and B, the vertical hydraulic conductivity could be on the order of 10^{-2} to 10^{-3} ft/d.

Data from Black, Crow, and Eidsness (1978) collected at the southwest St. Petersburg WRF injection site, show little difference between vertical and horizontal hydraulic conductivity in the semiconfining units. This data agrees with Stewart’s (1966) data from equivalent strata in Polk County, which also show little or no difference between vertical and horizontal conductivity.

WATER QUALITY

Freshwater, saltwater, and a mixture of the two occur in the rocks underlying St. Petersburg. Saline ground water predominates; freshwater typically occurs as a thin layer above the saltwater. Freshwater is maintained by recharge from rainfall that infiltrates the rocks underlying St. Petersburg. Sources of saline ground water are probably the Gulf of Mexico, Tampa Bay, and residual seawater from the geologic past (Hickey, 1982). Hydrodynamic dispersion or mechanical mixing is the dominant process associated with the spreading of the solute.

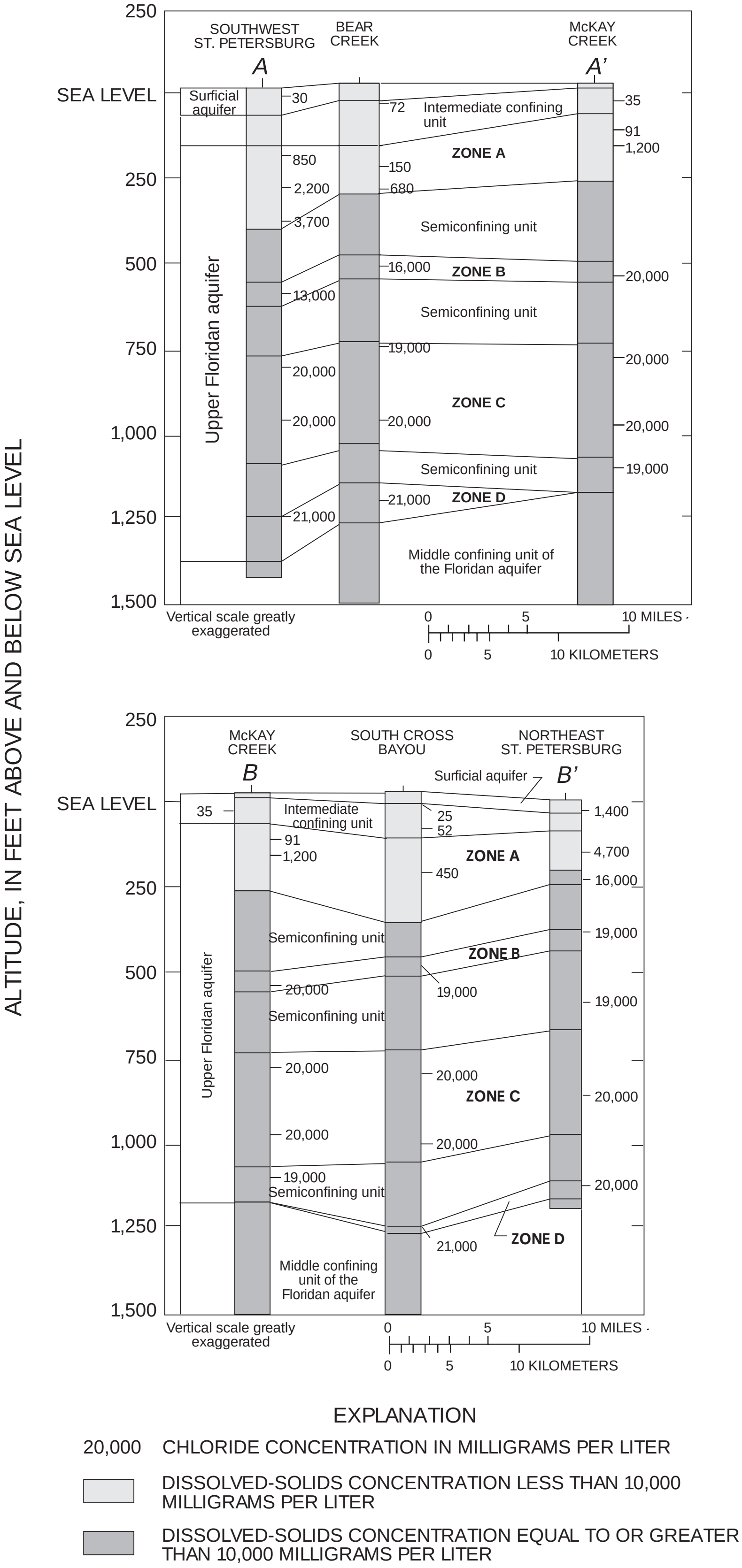


Figure 3. Vertical sections A-A' and B-B' showing chloride and dissolved-solids concentration in ground water. (Modified from Hickey, 1982.)

Native Ground Water

Water within the Upper Floridan aquifer is more mineralized than water from the surficial aquifer. Figure 3 shows vertical and lateral profiles of chloride and dissolved solid concentrations in ground water along lines A-A' and B-B'. Chloride concentrations in water from the surficial aquifer range from 30 to 1,400 mg/L. Chloride concentrations in water from zone A range from 91 to 16,000 mg/L and in water from zones B through D from 13,000 to 21,000 mg/L. Water in zones C and D is comparable to seawater.

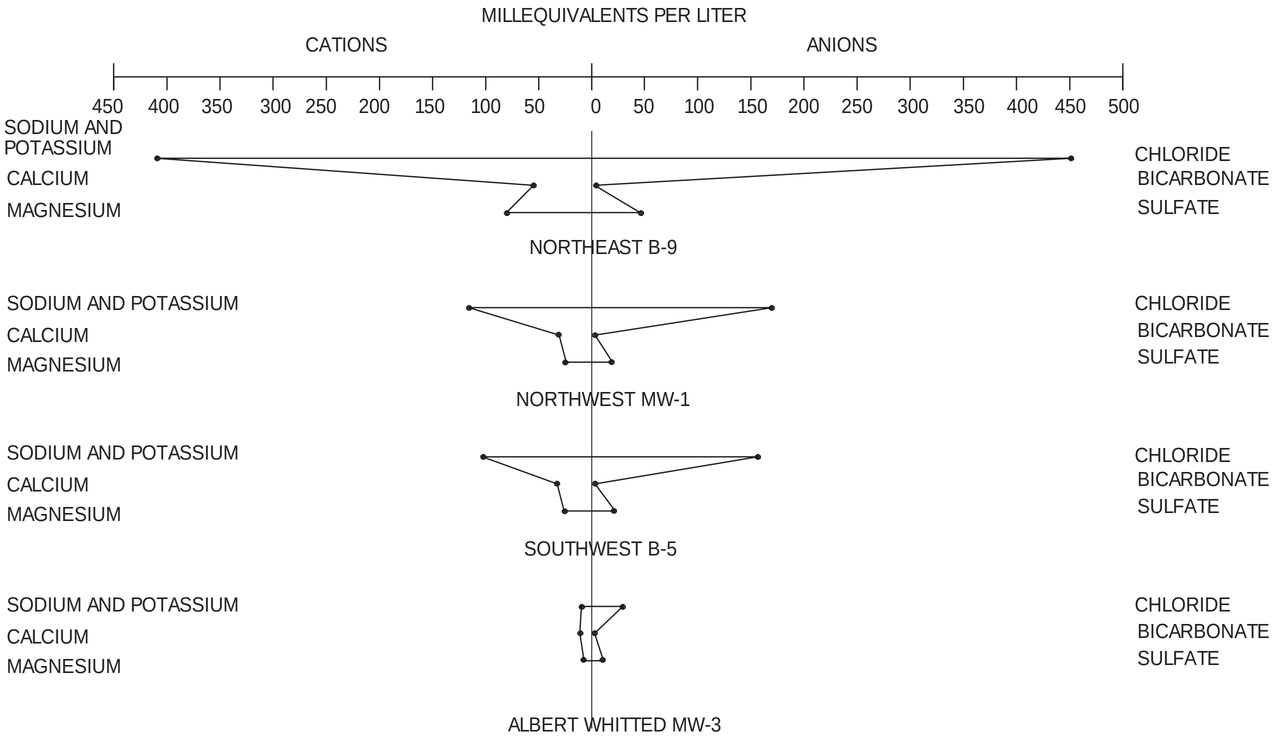
The salinity of water within rocks comprising zone A varies both vertically and areally. Freshwater, where present, is typically in a thin lens at the top of the zone. Dissolved-solids concentrations increase with depth. Ground water near the coastal margins of St. Petersburg have higher concentrations in both the upper and lower parts of zone A. The vertical variation in water quality suggests that water in zone A is density stratified (Hickey, 1982).

Water-quality characteristics of zone A at each of the city's four WRF's are shown in table 1 (CH2M Hill, 1993). Most water in zone A is slightly to moderately saline with DS concentrations ranging from 2,520 to 32,900 mg/L. Waters of zone A generally are a sodium choride type (fig. 4).

Effluent

Effluent at each of the city's four WRF's is aerated, filtered, and chlorinated reclaimed wastewater. The water quality of the effluent is variable due to differences in the influent (incoming waste) and the treatment processes at each WRF (table 1). The average pH is about 7 and the effluent contains low concentrations of suspended solids (less than 3.0 mg/L). The DS and chloride concentrations range between about 400 to 900 mg/L and about 125 to 350 mg/L, respectively. All waters are a sodium chloride type (fig. 4).

A. WELLS OPEN TO ZONE A



B. EFFLUENT

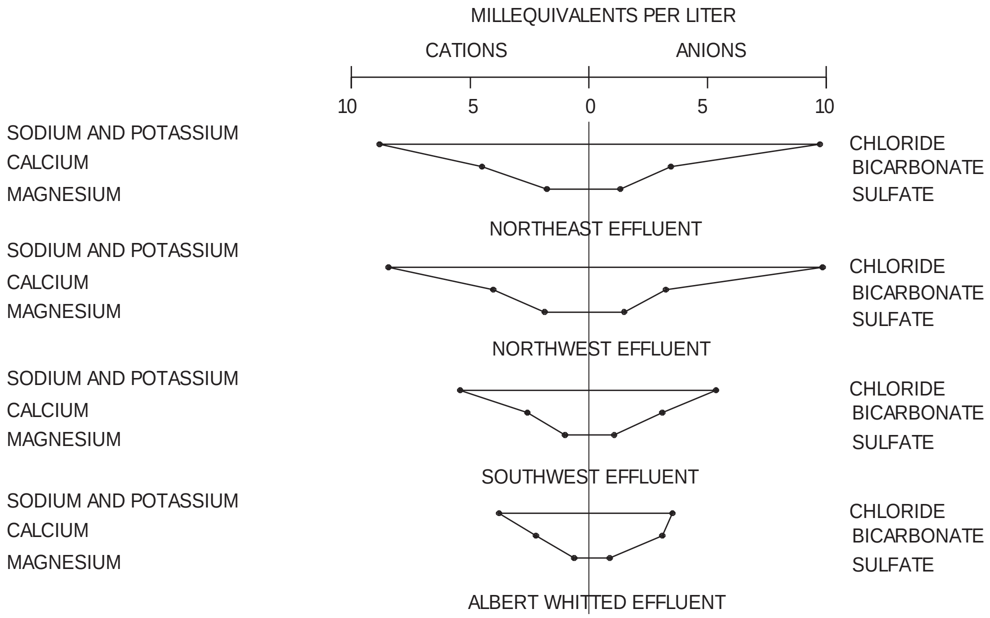


Figure 4. Chemical composition of water at the city of St. Petersburg's water reclamation facilities. (A) selected wells open to zone A, and (B) effluent.

Table 1. Chemical composition and saturation indices of ground water from zone A and effluent at the city of St.Petersburg water reclamation facilities

[<, less than, --, no data. Chemical analysis expressed in milligrams per liter except as noted; ^{o}C, degrees Celsius; µS/cm, microsiemens per centimeter]

	Ground water				**Effluent**[2]			
	Northeast well B-9[1]	**Northwest well MW-1**[2]	**Southwest well B-5**[2]	**Albert Whitted well MW-3**[3]	**Northeast**	**Northwest**	**Southwest**	**Albert Whitted**
Parameter								
Temperature (^{o}C)	26.2	24.7	24.9	--	25.2	25.5	25.8	26.4
Specific conductance (µS/cm)	44,800	17,800	22,400	4,400	1,613	1,610	1,100	844
Dissolved solids	32,900	11,600	11,400	2,520	888	882	574	412
pH (units)	6.7	7.03	6.88	7.17	6.92	7.15	7.16	7.17
Calcium (Ca)	1,100	623	653	229	90.3	80.8	52.0	44.8
Magnesium (Mg)	980	296	318	84.8	21.6	22.7	12.3	7.62
Sodium (Na)	9,300	2,640	2,350	222	197	187	119	83.1
Potassium (K)	200	34	29	10.5	9.8	12	9.7	6.9
Chloride (Cl)	16,000	6,040	5,540	1,050	345	349	190	125
Sulfate (SO_4)	2,200	938	1,060	546	63.7	71.5	51.2	42.2
Bicarbonate (HCO_3)	160	202	188	161	211	198	189	189
Fluoride (F)	0.0	0.29	0.35	0.23	0.64	0.60	1.03	0.77
Total nitrogen (N)	0.61	3.3	3.4	--	12.9	11.6	8.2	19.4
Total phosphorous (P)	0.26	<0.04	<0.01	--	1.66	0.64	1.57	0.43
Saturation indices[4]								
Calcite	-0.258	0.154	-0.003	0.001	-0.351	-0.339	-0.192	0.360
Dolomite	-0.146	0.361	0.061	-0.063	-0.966	-0.942	-0.575	-1.121
Anhydrite	-0.441	-0.725	-0.647	-0.958	-2.005	-2.229	-1.993	2.325
Aragonite	-0.400	0.010	-0.147	-0.143	-0.495	-0.482	-0.336	-0.503
Gypsum	-0.251	-0.509	-0.432	-0.741	-1.789	-2.020	-1.780	2.121

[1] Chemical analyses from Hickey, 1982, table 5.

[2] Chemical analyses from CH2M Hill, 1993, table 5.2.

[3] Chemical analyses from Post, Buckley, Schuh & Jernigan, Inc., 1989, appendix 6.

[4] Log [ion activity proudct/equilibrium constant].

Geochemical Interactions

The injection of water into an aquifer having water of different quality than the injected water may change local conditions, resulting in geochemical interactions that lead to changes in water-quality and aquifer properties. Mixing of two waters of different chemical character may produce chemical reactions that could precipitate minerals, thus, reducing transmissivity and porosity; dissolve minerals, thus, increasing transmissivity and porosity, or the injected water may be in equilibrium with the aquifer minerals and native water, resulting in no chemical reactions.

The potential for a chemical reaction can be determined by calculating the chemical equilibrium of the injected and aquifer waters. The equilibrium state of the water with respect to a mineral phase can be determined by calculating a saturation index (SI) using analytical data. The SI is defined as the logarithm of the ratio of the ion activity product to the mineral equilibrium constant at a given temperature. If SI is equal to zero (0), the water is in equilibrium with the mineral; if it is less than 0, the water is undersaturated and if present, that mineral will dissolve; if the ratio is greater than 0, the water is supersaturated and mineral precipitation would be possible. Because of uncertainties in analytical and thermodynamic constants, a water with a SI value between 0.1 and -0.1 is assumed to represent saturation conditions or is in equilibrium with respect to the mineral phase (Swancar and Hutchinson, 1992).

The SI for the resident native waters and for the effluent, with respect to minerals commonly found in carbonate aquifers, was calculated using the computer program WATEQF (Plummer and others, 1976) and values are given in table 1. The values in table 1 show that most of the native ground water is saturated to supersaturated with respect to calcite and dolomite, and undersaturated with respect to the remaining minerals. The ground-water sample for the northeast WRF was undersaturated with respect to calcite and dolomite. This water has a very high concentration of DS and probably is residual seawater. The effluent is undersaturated with respect to all minerals; therefore, these waters apparently could dissolve minerals including calcite and dolomite, the principal minerals that compose carbonate aquifers.

The mass-balance model PHREEQE (Parkhurst and others, 1980) was used to simulate the geochemical reactions that may occur when effluent is mixed with native ground waters. PHREEQE is a generalized aqueous speciation, solubility, mass-transfer computer code that can simulate several types of reactions including the mixing of two waters of different chemical compositions. Modeled reactions were evaluated based on the equilibrium state of a 50 percent mix of the two water types with respect to selected mineral phases. Two simulations were made: The first model run simulated effluent from the Albert Whitted WRF entering the aquifer monitored by well MW-3. The second model run simulated effluent from the southwest WRF entering the aquifer monitored by well B-5. Results of the simulations indicate that the mixed effluent and ground water would be undersaturated with respect to all minerals (table 2). These data infer that the injected effluent, upon entering the aquifer and mixing with the aquifer waters, may dissolve calcite and dolomite. This process could produce a more porous limestone with increased transmissivity.

Table 2. Selected saturation indices from PHREEQE model results

Saturation indices	Model 1 [1]	Model 2[2]
Calcite	-0.459	-0.122
Dolomite	-1.185	-0.068
Anhydrite	-2.324	-1.005
Aragonite	-0.645	-0.309
Gypsum	-2.116	-0.794

[1] Effluent at Albert Whitted facility entered the aquifer monitored by well MW-3.

[2] Effluent at Southwest facility entered the aquifer monitored by well B-5.

SIMULATION OF SUBSURFACE STORAGE AND RECOVERY OF TREATED EFFLUENT

A finite-difference cylindrical-flow model of ground-water movement and solute transport was used as a simulation tool to determine the recovery efficiency of a prototype SSR system for a moderately transmissive, slightly to moderately saline aquifer, underlying St. Petersburg. Specific questions to be answered are: (1) In what quantitative fashion will the physical and operational variables influence recovery efficiency?, and (2) Will recovery efficiency improve when SSR is conducted as a multiple-cycle operation?

To answer these questions, HST3D was used to simulate a well in a hypothetical hydrogeologic section representing St. Petersburg. The analysis implemented a conceptual modeling approach (Merritt, 1985), in comparison to a calibration and predictive approach (Merritt,1994), as no data exist for comparison with model results. This type of analysis permitted many combinations of conditions that could be investigated using parameters generally similar to those of the aquifer system underlying St. Petersburg. Sensitivity tests were used to examine the response of the model to a range of hydrogeologic and fluid properties and the effect of various injection/withdrawal schemes on the recovery efficiency of the SSR system.

Numerical Model

The HST3D model (Kipp, 1987) is a computer program written in FORTRAN-77 that simulates variable density fluid movement and transport of either dissolved substances or energy in the subsurface. The model, as used in this report, solves for two interdependent variables: pressure and mass-fractional concentration in cylindrically symetrical coordinates under isothermal conditions. Backward-in-space and backward-in-time finite-difference equations were used for solution of ground-water flow and the solute-transport equations in the numerical model. The reader is referred to Kipp’s (1987) report for a complete discussion of the model code and numerical methods.

Design of Base Model

A base model used as a standard for comparisons for subsequent sensitivity analyses was designed to be representative of the slightly to moderately saline artesian limestone aquifer underlying St. Petersburg. Hydraulic and solute properties used in the model are representative of the city’s four WRF injection sites and, as such, do not represent any specific location in St. Petersburg. Data were obtained from previous studies and laboratory values reported in text books.

To apply the HST3D model, the hydrologic and hydrogeologic characteristics of the aquifer system in St. Petersburg was simplified into the rectangular section in figure 5. The cylindrical-flow base model simulates the intermediate confining unit, permeable zone A, and the lower semiconfining unit. It consists of 26 variable-width node spacings in the vertical direction and 88 variable-width node spacings in the radial direction. The model dimensions are 2,500 horizontal ft and 420 vertical ft. The vertical spacing ranges from 10 to 50 ft. Radial spacing expands logarithmically from 0.14 ft at the well up to a maximum of 50 ft. The base model was used as the reference for sensitivity testing.

Several simplifying assumptions were made in the conceptualization and simulation of the flow system:

1. The aquifer system is homogeneous and isotropic in all directions,
2. Hydrostatic conditions initially prevail,
3. Regional horizontal and vertical flow is negligible,
4. A uniform native fluid density exists within each model layer,
5. The water-quality profile is laterally homogeneous throughout the model area,
6. The viscosities of the injected and native fluids are the same, and
7. Dispersivity is constant throughout each model layer.

Model Parameters

The strategy for the model analysis was to choose parameter values that, even though nonunique, would approximate conditions representative of the system so that the major processes affecting the mass fraction distribution during injection and withdrawal would be simulated. The parameters simulated in the model include boundary conditions, matrix properties, fluid properties, and well characteristics. A description of each model parameter follows:

1. Boundary conditions.--Boundary conditions are used to constrain the lateral and vertical extent of the simulated flow system providing a simplified representation of the flow and transport processes at the model limits. The top and bottom boundaries of the model are specified pressure boundaries because the producing zones are very permeable relative to the entire Floridan aquifer system (Knochenmus and Thompson, 1991). Pressure on the upper boundary is set at 12.967 lb/in^2, equivalent to the pressure exerted from an overlying 30 ft column of freshwater presumed to exist in the overlying hypothetical surficial aquifer. Pressure on the lower boundary is 195.719 lb/in^2, equivalent to the pressure exerted from a 450-ft column of freshwater and saline water presumed to exist in the overlying formations. The inner radial edge is defined by

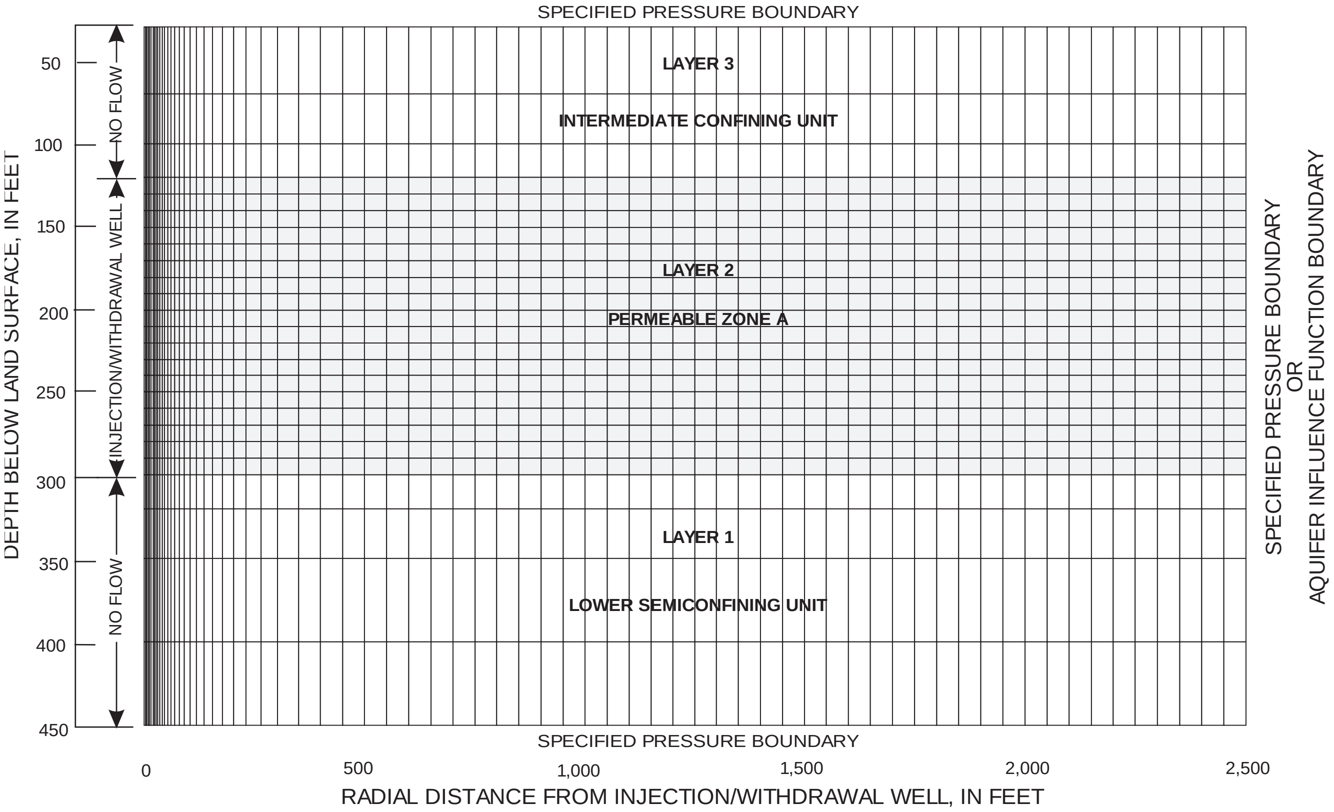


Figure 5. Radial-model grid, boundary conditions, and model layering.

the injection/production well in zone A and a no-flow boundary condition for the confining units above and below the well. The outer radial edge is specified pressure for the single 30-day test cycle and hydrostatic pressures at each node are based on a column of water having DS concentration specified as a function with depth. Water that enters the section at a given node as a result of a pressure gradient at the boundary is of specified concentration; water that exits at such a node is of ambient aquifer concentration. For the multiple-test cycles, the outer radial edge is defined by a transient flow, aquifer influence function (AIF). AIF utilizes the Carter-Tracy approximation (Kipp, 1987) to compute flow rates between the inner gridded aquifer region and an infinite homogeneous outer region where aquifer properties are known only in a general sense. The radius of the inner region was set at 2,500 ft and the outer region is modeled as an infinite cylinder with a height of 420 ft. Initial hydrostatic pressures throughout the model were set based on the boundary conditions.

2. Matrix properties.--Matrix properties are defined for each of the three hydrogeologic layers for the model in table 3. The porous media properties are intrinsic permeability, matrix compressibility, effective porosity, longitudinal dispersivity, and transverse dispersivity. Intrinsic permeability was calculated from hydraulic conductivity values reported by Hickey (1982), with conversion factors from Freeze and Cherry (1979, p. 29). Values of hydraulic conductivity and matrix compressibility were based on aquifer tests and laboratory tests of limestone samples collected during previous studies. The value of porosity used in this model, 0.3, is an estimate based on geophysical logs at the WRF injection sites in St. Petersburg. Longitudinal (α_L) and transverse (α_T) dispersivities of the system were set at 12.5 ft and 2.5 ft, respectively. Even though the spatial gridding stability rule-of-thumb criteria recommended in Voss (1984, p. 232), suggest that α_L and α_T be greater than one-fourth and one-tenth of the radial and vertical spacings, an acceptable solution was computed using an α_T value equal to 2.5 ft.

Table 3. Fluid and matrix properties assumed for simulation

[°F, degrees Fahrenheit; lb/ft^3, pounds per cubic foot; in^2/lb, inch squared per pound; ft^2/d, foot squared per day; ft/d, foot per day; ft^2; foot squared]

Parameter	Lower semi-confining unit	Zone A	Intermediate confining unit
Fluid properties			
Temperature (°F)	75.0	75.0	75.0
Specific weight (lb/ft^3)	63.177	62.468	62.241
Viscosity (centipoise)	0.8904	0.8904	0.8904
Fluid compressibility (in^2/lb)	$3.03E^{-6}$	$3.03E^{-6}$	$3.03E^{-6}$
Molecular diffusivity (ft^2/d)	$9.30E^{-5}$	$9.30E^{-5}$	$9.30E^{-5}$
Scaled mass fraction	1.0	0.25	0.025
Matrix properties			
Hydraulic conductivity (ft/d)	1.0	167.0	$8.0E^{-4}$
Intrinsic permeability (ft^2)	$3.877E^{-12}$	$6.475E^{-10}$	$3.102E^{-15}$
Porosity (unitless)	0.3	0.3	0.3
Longitudinal dispersivity (feet)	12.5	12.5	12.5
Transverse dispersivity (feet)	2.5	2.5	2.5
Matrix compressibility (in^2/lb)	$6.2E^{-6}$	$6.2E^{-6}$	$6.2\ E^{-6}$

3. Fluid Properties.-- The fluid properties of the native formation water assumed for the simulations are listed in table 3 and include temperature, specific weight, viscosity, compressibility, molecular diffusivity, and DS expressed as scaled-solute mass fraction (SSMF). The model was simplified with the assumption of a vertically uniform initial DS concentration distribution assigned to each layer although a vertical salinity gradient has been documented. Isothermal conditions at 75°F were assumed to prevail. Fluid densities assigned to injected and native waters were based on the measured or estimated concentration of DS in each fluid. Viscosity of the injected and native formation waters vary with temperature and solute fraction. Because isothermal conditions were assumed to prevail and because the viscosity of freshwater and saltwater differ by only 0.06 centipose, viscosity was assumed invariant in the simulations. The assigned value of viscosity was held constant at 0.8904 centipose (viscosity of pure water at 75°F). Compressibility of water was held constant at 3.03×10^{-6} in^2/lb (Freeze and Cherry, 1979, p. 52), and molecular diffusivity of the solute in the porous media was set at 9.30×10^{-5} ft^2/d (Kimbler and others, 1975). The model SSMF is a dimensionless relative solute-concentration term ranging in value from 0 to 1. Any fluids present within the aquifer system, or entering it in simulation exercises, are considered to be a mixture of the two fluids by the appropriate specification of SSMF values. SSMF = 0 was used to represent pure freshwater, and SSMF = 1 represents the most saline water residing within the aquifer system, that in the lower confining unit. The assigned densities of 62.241 lb/ft^3 (SSMF = 0) and 63.177 lb/ft^3 (SSMF = 1) at 75°F and atmospheric pressure were obtained from a standard handbook (Chemical Rubber Company, 1982). The SSMF values of the injected effluent, the water of the aquifer system, and water in mixtures of effluent and native formation waters are assigned based on their salinity relative to the two extremes. SSMF values of 0.025 (500 mg/L DS) and 0.25 (5,000 mg/L DS), representing the composite background water quality collected at the WRF injection sites, were assigned to the intermediate confining unit and zone A, respectively, based on the ratio of DS concentration to the estimate DS concentration of the lower confining unit. Measured injected-water DS concentration was about 700 mg/L and was assigned a SSMF value of 0.035.

4. Well information.--The well occurs at the first column of nodes and the open-hole interval of the well is defined by row numbers. Injection and withdrawal of effluent is through 18 nodes distributed vertically which, when combined, represent permeable zone A (180-ft interval). Injection and withdrawal flow at the well bore is allocated over rows 5 to 23 by mobility factors that are based on cell position, relative hydraulic conductivity, and an element completion factor. An element completion factor of 0 means the well is cased off from the aquifer in that element, whereas an element completion

factor of 1 means equivalent flow across the cell length.

Effects of Hydrologic Parameter Variations on Recovery Efficiency

When the results of a simulation study are largely based upon assumed estimates of data rather than measured data, as in this case, determining the effect of parameter variations on simulation results is of particular interest. To learn which properties and conditions substantially affect recovery efficiency, a series of simulation runs were made that started with the base model. For each simulation run, the value of an individual model parameter was changed by an amount that it might reasonably be expected to vary from the value used in the base simulation, then noting the change in recovery efficiency as a result of the change. The base simulation used as a standard for comparison consisted of a single cycle of 15 days of injection of effluent at a rate of 1.0 Mgal/d at a temperature of 75°F and a maximum of 15 days of withdrawal at a rate of 1.0 Mgal/d. Thus, one injection/withdrawal cycle is completed in 30 days. Withdrawal was assumed to end when the increasingly saline water exceeded the maximum DS concentration (1,500 mg/L) deemed acceptable for irrigation use. For the base model, a DS concentration of 1,500 mg/L was reached in 3 days. The recovery efficiency calculated for the base model single 30-day cycle simulation is 20.0 percent.

The effect of parameter changes on recovery efficiency is presented in the following sections. Discussion of individual parameters is ordered from most to least sensitive.

Resident Fluid Dissolved-Solids Concentration of Zone A

A series of sensitivity tests were used to show the relation between recovery efficiency and resident fluid DS concentration of the injection zone (zone A). Two resident fluid DS concentrations of zone A were selected for comparison with the 5,000 mg/L base value: (1) 2,300 mg/L, an arbitrary value representing water somewhat less saline than the composite base value, and (2) 20,000 mg/L, representing the most saline layer in the model. Relations were established for a range of α_L and α_T combinations. DS concentrations simulated for the base model were 500 mg/L for the intermediate confining unit, 5,000 mg/L for zone A, and 20,000 mg/L for the lower semiconfining unit.

Because of the lack of local field data to indicate the degree of dispersion in the carbonate system, three additional dispersion values (sets of longitudinal α_L and transverse α_T dispersivities representing some hypothetical degree of dispersion) were chosen to compare to the dispersion used in the base model. The additional dispersion values used for analysis are summarized below:

Dispersion value set	α_L (ft)	α_T (ft)
1	4.0	1.0
2	25.0	1.0
3	25.0	5.0

Dispersion value set 1 is a low degree of dispersion in the radial flow direction and a low degree of interlayer dispersion. Value set 2 introduces an appreciable degree of dispersion in the radial flow direction. Value set 3 represents appreciable degrees of dispersion in the radial flow direction and between layers.

Figure 6a shows the decline of recovery efficiencies with increasing resident fluid DS concentration for the various dispersivity combinations. The larger the DS difference between the injected water and resident formation water, the less efficient the SSR process. Recovery efficiency was shown by the model to be significantly less in aquifers of high salinity than in slightly saline aquifers. With higher resident fluid DS concentration, less water within the zone of mixing is acceptable for withdrawal. Higher DS concentrations also make density stratification of the fluids more likely to occur at a given permeability level, decreasing recovery efficiency. Recovery efficiency was shown to be greater when the level of dispersive mixing decreased, or such as when a smaller volume of injected fluid combines with more saline native formation water. Thus, recovery efficiency is most promising when resident fluid DS concentrations are low, and least promising when DS concentrations are high.

Dispersivity

Dispersivity is a scale-dependent property of the porous medium that controls the mixing of injected and resident formation fluids at their interface. When dispersivities are increased, there is more mixing that results in a widening of the transition zone between the injectant and native formation waters.

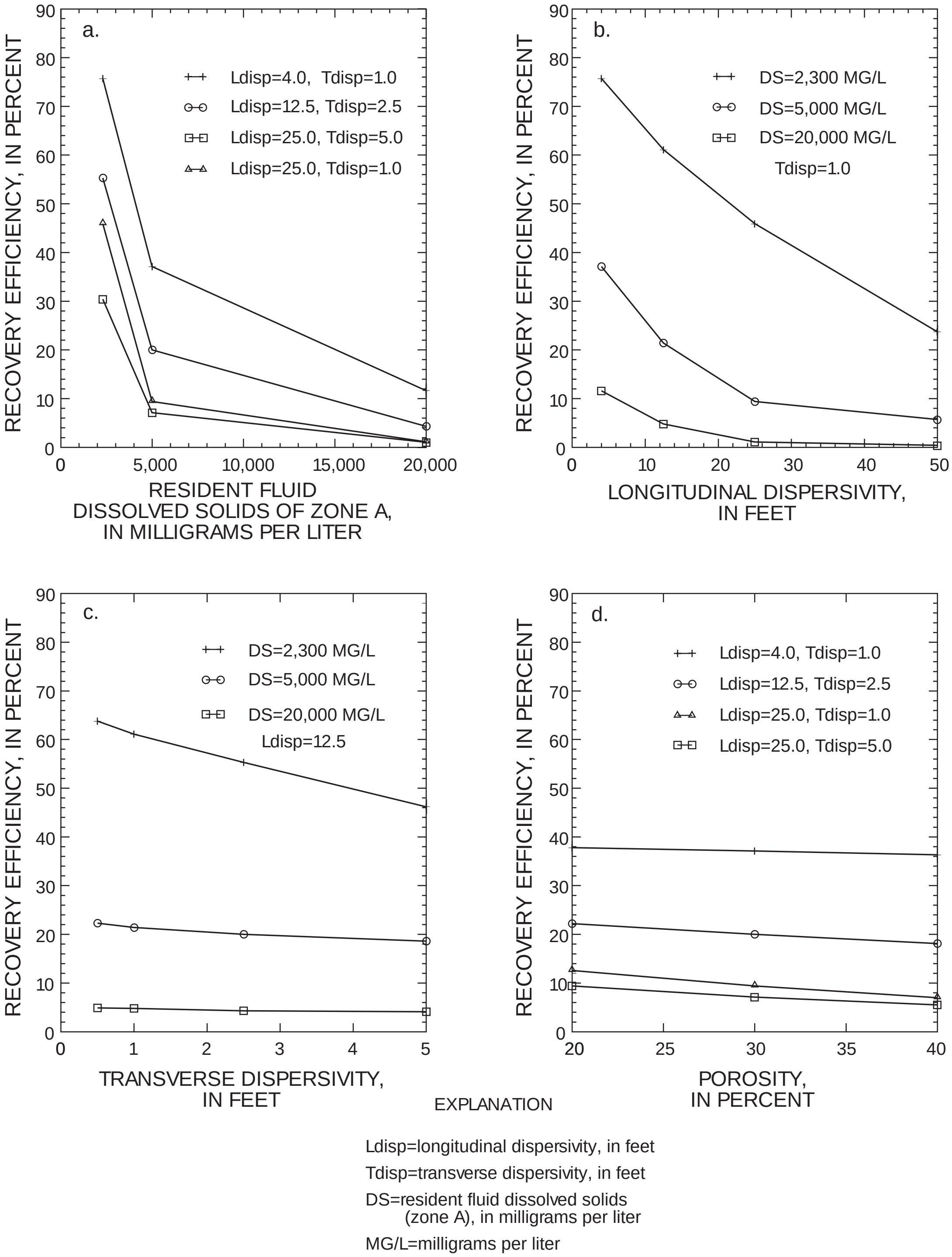


Figure 6. Relation between recovery efficiency and variations in selected model parameters.

Dispersion is a deleterious process that can severely limit recovery efficiency. Merritt (1985) reported that recovery efficiency is limited when the upper limit of the concentration of some constituent considered acceptable in recovered water is less than half of the average concentration of the injected and native formation waters. In the hypothetical test case posed in this analysis, the acceptable limit for DS concentration (1,500 mg/L) was equal to or less than the average of the injected water (700 mg/L) and the native water (2,300 to 20,000 mg/L).

Various values of dispersion in the direction of flow (longitudinal) and interlayer (transverse) were tested. Values of α_L were varied between 4 and 50 ft with respect to 12.5 ft in the base model, and values of α_T were varied between 0.5 and 5.0 ft with respect to 2.5 ft in the base model, when the rate and duration of injection and withdrawal was kept constant.

Figure 6b and c illustrates the results from the analysis for the three previously cited resident fluid DS concentrations (2,300, 5,000, and 20,000 mg/L). Results show the decline of recovery efficiency as the dispersivity value increases. A large decrease of recovery efficiency is shown as α_L increases from low values of α_L, but the rate of decrease is small at larger values of α_L. Recovery efficiency was slightly affected by changes in α_T at low ranges of the parameter but at higher ranges, recovery efficiency was relatively unaffected by its variation. Evidently, for every resident fluid TDS concentration, there are values of α_L and α_T above which recovery efficiency is significantly reduced

Porosity

Porosity of the injection zone (zone A) was tested at 0.2 and 0.4 to bracket the base model value of 0.3. Permeability and porosity control the velocity of injectant flow and, hence, the rate of solute transport. The greater the porosity, the slower the solute front will move; thus, the longer the time it takes to replace the volume of native formation water in a given volume of aquifer and the greater the dispersive mixing. Low porosity has the opposite effect.

Figure 6d illustrates the variation of recovery efficiency due to porosity changes in relation to the four previously cited dispersivity combinations. Increasing porosity caused recovery efficiency to decrease slightly for each dispersion model. Recovery efficiency decreased significantly, however, as the level of dispersive mixing increased.

Horizontal and Vertical Permeability of Zone A

The permeability of the aquifer material and the density contrast of the injected and native water determines whether an appreciable level of density stratification or buoyancy flow can occur. Density stratification refers to the physical process in which less dense injected fluid rises and flows over the more dense fluid. Generally, low permeability reduces stratification and optimizes recovery efficiency.

Values of horizontal (k_h) and vertical (k_v) permeability were changed simultaneously by the same factor that ranged from 0.1 to 10, with all other parameters remaining the same. The ratio of k_h to k_v was held to 1. Results of the simulations are as follows:

k_h and k_v (multiplier)	Recovery efficiency (percent)
0.5	19.8
1.0	20.0
2.0	19.5
5.0	15.7
10.0	7.7

When permeability was doubled or halved, recovery efficiency was not affected. The major effect of the variation at these permeability values was the wellhead pressure required at the specified injection/withdrawal rate. However, when permeability was made 10 times greater, recovery efficiency was reduced by 61.5 percent. This is because simulation of a larger permeability allowed for easier horizontal and vertical transport of the injected fluid, which resulted in greater stratification and buoyancy flow that prevented complete mixing of the injected water with the native water. Upon withdrawal, a greater percentage of native water was immediately available to the well.

Ratio of Horizontal to Vertical Permeability

If flow conditions vary with direction in a geologic formation, the formation is anisotropic and differences in horizontal (k_h) and vertical permeability (k_v) can influence fluid movement. The greater the anisotropy ratio (k_h/k_v), the easier the salt front moves along the axis with the larger permeability component which contains the injected water within the open interval of the injection well. In the base model, permeability is equal in all directions. Anisotropy in the model only can be simulated by varying the ratio of k_h to k_v. To test for the effects of anisotropy on model results the ratio of k_h to k_v was varied from an isotropic base condition ($k_h/k_v = 1$) to kh/kv equal to 100. Results of the simulations are as follows:

k_h/k_v	Recovery effciency
1	20.0 percent
10	21.9 percent
100	23.6 percent

Simulation of different values of k_h/k_v had a small affect on computed recovery efficiencies. Increasing k_h/k_v caused recovery efficiency to increase slightly. This is because simulation of a larger k_h/k_v causes more lateral flow and inhibits upward movement of buoyant injectant.

Effects of Operational Factors on Recovery Efficiency

The success of a SSR system is determined by the quantity of injected water that can be recovered from an aquifer. The sensitivity analyses indicated the physical and chemical parameters that substantially affect recovery efficiency. In addition to these parameters, operational factors also will affect the recovery efficiency of the SSR system. These factors include the duration and rate of injection and withdrawal, plus well construction. A series of model simulations was performed to evaluate the response of the model to changes in these factors. The base values of hydraulic and fluid properties were used in all simulations. Modifications were made to the HST3D model to simulate the shutdown of the production well when the solute fraction of the withdrawn water reached 0.0745, corresponding to a DS concentration of 1,500 mg/L. The production well was shutoff until the scheduled beginning of the next simulation.

Duration of Injection and Withdrawal Cycle

Two series of multicycle model simulation tests were used to illustrate the effects of variations in the duration of injection/withdrawal cycles on recovery efficiency. The first series of tests consisted of 3 simulations of five uniform successive cycles (60, 180, and 365 days) of injection and withdrawal of 1.0 Mgal/d. The following schedules were simulated:

1. 30 days of injection followed by a maximum of 30 days withdrawal
2. 90 days of injection followed by a maximum of 90 days of withdrawal
3. 183 days of injection followed by a maximum of 182 days of withdrawal

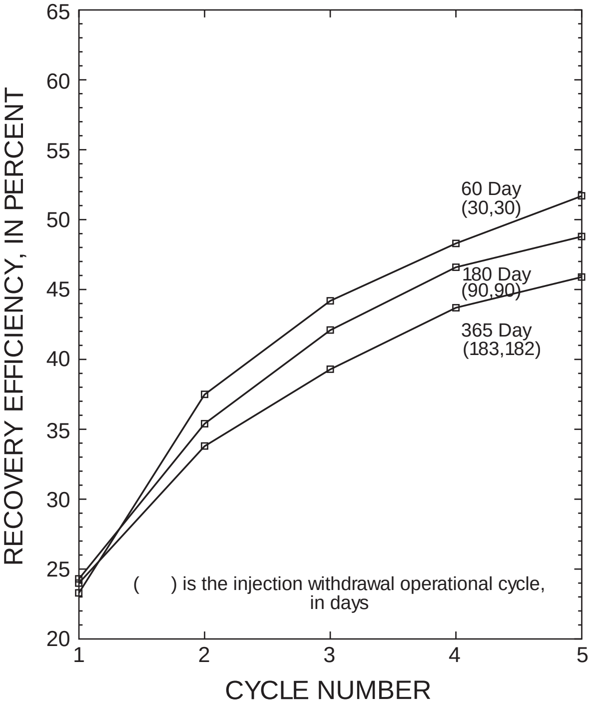


Figure 7. Recovery efficiencies for five successive 60-, 180-, and 365-day injection/withdrawal cycles at 1.0 million gallons per day. (Withdrawal in each cycle ceases when the dissolved-solids concentration of withdrawn water exceeds 1,500 milligrams per liter.)

Figure 7 shows the results of the first series of testing cycles for five successive 60-, 180-, and 365-day cycles. The plot indicates that recovery efficiency improves with each successive cycle for the various operational schemes even if the volume of injectant does not increase. This is because of the continuous growth of the zone of dispersion (mixing zone) and the retarding effect of the zone of dispersion on the rate of gravitational segradation (Kumar and Klimbler, 1970). With each cycle, the zone of dispersion is greater due to mixing of the injectant with the residual water that was not completely recovered from the previous cycle. The graph also shows recovery efficiency increasing very rapidly in intitial cycles and then more slowly at later cycles for each operational schedule. After five cycles, recovery efficiencies ranged between 46 and 52 percent. Recovery efficiencies at the end of the first cycle had ranged between 23 and 24 percent.

Higher recovery efficienies were obtained for simulation tests when the duration of injection and recovery phases was shorter. This is expected because of the nature of the conceptual system in which migration of the solute particles across the low permeable units will reduce the recoverability for tests of longer duration (Quinones-Aponte and Wexler, 1995).

An operational SSR system would not function on uniform cycles but rather on irregular cycles based on seasonal surplus and demand. In the second series of tests, a hypothetical yearly schedule of injection and withdrawal was simulated. The schedule consisted of five successive 1-year cycles of 4-months of injection, followed by a maximum of 3-months of withdrawal, followed by 3-months of injection, and finally followed by a maximum of 2 months of withdrawal. In St. Petersburg, the injection periods correspond to December through March and July through September (months when irrigation reuse is low), and the withdrawal periods might correspond to April through June and October through November (months when irrigation reuse is high).

Figure 8 shows the results of the second series of tests. The model conditions are similar to those previously described for the five successive 60-, 180-, and 365-day cycles. Recovery efficiencies range between 27 and 47 percent for the 0.5 Mgal/d simulations, 31 and 55 percent for the 1.0 Mgal/d simulations, and 37 and 62 percent for the 2.0 Mgal/d simulations. Results indicate that recovery efficiency approach an asymptote after several cycles, where for practical purposes, no improvement of recovey efficiency occurrs. For the 2.0 Mgal/d simulation the maximum recovery efficiency probably will be between 65 and 70 percent.

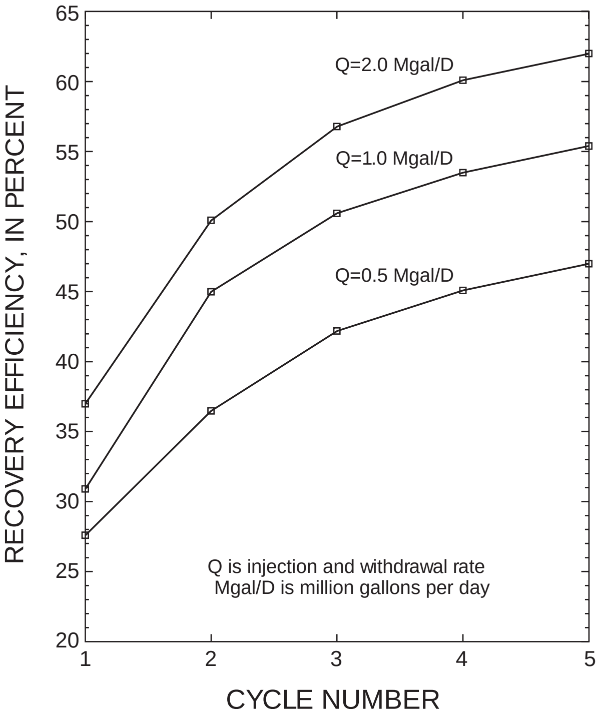


Figure 8. Recovery efficiencies for five successive 1-year cycles of 121 days of injection, 91 days of withdrawal, 92 days of injection, and 61 days of withdrawal at rates of 0.5, 1.0, and 2.0 million gallons per day. (Withdrawal in each cycle ceases when the dissolved-solids concentration of withdrawn water exceeds 1,500 milligrams per liter.)

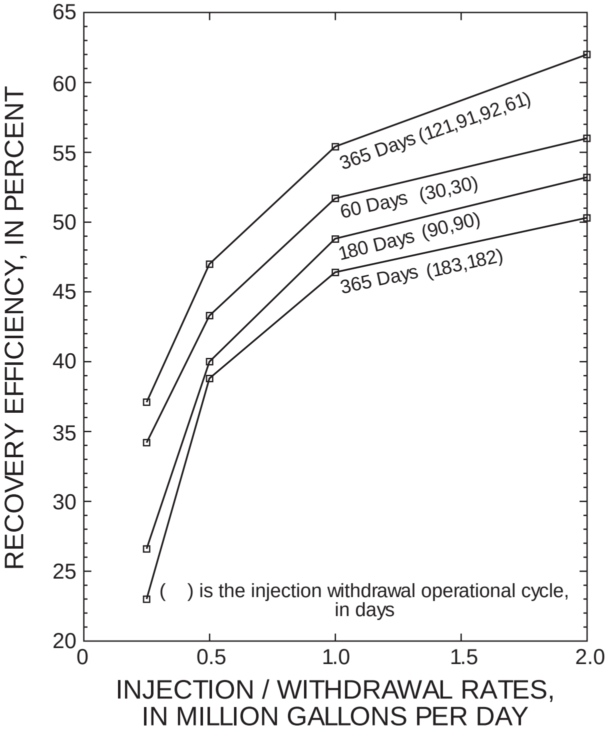


Figure 9. Recovery efficiencies after five cycles for various injection/withdrawal rates and operational schemes.

Rate of Injection and Withdrawal

The rate of injection and withdrawal for a fixed time period and for various operational schemes was varied from 0.25 and 2.0 Mgal/d to determine whether certain injection/withdrawal rates favor higher recovery efficiencies. Zero recovery efficiency would occur for a sufficiently small injection volume because of mixing. Results of the tests suggest that recovery efficiency is directly proportional to the injected flow volume. For a given operational scheme, recovery efficiency increases with higher volumes (fig. 9). There is a larger rate of increase of recovery efficiency at smaller volumes than at larger volumes. Recovery efficiencies after five cycles ranged between 50 and 62 percent for an injection/withdrawal rate of 2.0 Mgal/d and between 23 and 37 percent for an injection/withdrawal rate of 0.25 Mgal/d.

Partially Penetrating Well

Several well-completion designs were simulated to evaluate the effects of partial penetration. Operational wells may be open only to part of an aquifer; thus, it is of interest to compare the recovery efficiency of a partially penetrating well with recovery efficiency of a well open to the full thickness. The recovery efficiency was expected to be higher in partially penetrating wells than for fully penetrating wells because a buffer zone of fresher water would exist between the pumped zone and the underlying water of poor quality. The simulated well penetrations ranged from 100 to 25 percent. The 25-percent penetration well is open to the upper 45 ft of layer 2. Results of the simulations are shown below:

Well penetration (percent)	Recovery efficiency (percent)
100	20.0
75	22.3
50	23.4
25	24.1

Simulations show a slight increase in recovery efficiency with a decrease in penetration depth. Merritt (1985) reported similiar results and suggests that recovery efficiencies in stratified aquifers may not be significantly affected if the well is open only to part of the aquifer. However, to generalize these results, a more-detailed study focusing on this aspect (injection into different flow zones) is needed.

SUMMARY AND CONCLUSIONS

A model-based study of the confined saline aquifer system underlying St. Petersburg is being conducted to analyze the hydrogeologic and operational aspects of underground injection, storage, and withdrawal of advanced secondary treated effluent in a single representative well. The study is specifically aimed toward (1) defining the hydrogeologic framework and ground-water quality in the study area, (2) assessing the geochemical interactions associated with the injection of effluent, and (3) applying a density-dependent, ground-water flow and solute-transport model to understand the relative importance of physical and chemical properties and operational variables on recoverability of injected effluent.

The sediments underlying the study area form a layered sequence of two aquifers and one confining unit. The framework includes the unconfined, surficial aquifer, and the confined Upper Floridan aquifer. The units are separated by the intermediate confining unit.

The surficial aquifer is composed of a layer of clastic deposits that is generally less than 30 ft thick. The aquifer is a source of recharge to the Floridan aquifer system and is primarily used as a source for lawn irrigation.

The intermediate confining unit is composed of clastic and carbonate sediments of Miocene and younger age. The carbonates are generally underlain and overlained by clays of relatively low permeability. Thickness of the unit averages about 90 ft and ranges from about 50 to 140 ft. The vertical hydraulic conductivity of the unit ranges from about 1.3 x 10^{-4} to 6.9 x 10^{-3} ft/d.

The Upper Floridan aquifer consists of a thick, regionally extensive sequence of Tertiary-aged carbonate rocks that comprise the following formations (in ascending order): Avon Park Formation, Ocala and Suwannee Limestones, and the Tampa Member of the Arcadia Formation which is part of the Hawthorn Group. The Upper Floridan aquifer underlying St. Petersburg contains four permeable zones separated by semconfining units. The zones are alphabetically labeled with increasing depth from A to D. The proposed receiving zone is within the uppermost part of the Upper Floridan aquifer (zone A) in the permeable limestone section of the Tampa Member of the Arcadia Formation of the Hawthorn Group and the Suwannee Limestone. Thickness of zone A averages about 180 ft and ranges from about 115 to 245 ft. Transmissivity of zone A ranges from 2.2 x 10^4 to 3.5 x 10^4 ft^2/d.

A semiconfining unit within the Suwannee Limestone is below the proposed injection zone and has a vertical hydraulic conductivity estimated to range from about 0.1 to 1.0 ft/d where the beds do not contain clay. Average thickness of this unit below the proposed injection zone is about 150 ft.

Limited fresh ground-water supplies exist in the Upper Floridan aquifer underlying St. Petersburg. Fresh ground water, where it is found, typically occurs as a thin layer within the uppermost permeable zone. Most water in the aquifer is saline with chloride concentration in the proposed injection zone ranging from 91 to 16,000 mg/L.

The chemical contrast between the injection and resident formation waters may lead to chemical reactions. The mix of the two water types would be understaturated with respect with calcite and dolomite. This might lead to dissolution of calcite and dolomite producing a more porous limestone with increased transmissivity.

A numerical model of variable density groundwater flow and solute transport (HST3D) was used to evaluate the importance of parameter variations affecting the recovery of effluent stored in a saline aquifer underlying the study area. The analyses consisted of a sensitivity testing approach, as opposed to the more familiar site-specfic calibration and prediction objective of modeling. Cyclic injection in a prototype aquifer was simulated and recovery efficiencies were calculated.

Sensitivity analyses were performed to determine changes in recovery efficiency when physical and chemical parameters of a base model are varied. The simulation cycle used as a standard for comparisons consisted of 15 days of injection of effluent at a rate of 1.0 Mgal/d and 15 days of withdrawal at a rate of 1.0 Mgal/d.

On the basis of computer simulations for hypothetical aquifer conditions, sensitivity tests for individual physical and chemical properties indicate:

1. The greater the density difference between the injected effluent and resident formation water, the lower the recovery efficiency during the first cycle. Higher salinity makes density stratification of the fluids more likely to occur at a given permeability level, thereby causing recovery efficiency to decrease.
2. Recovery efficiency decreases significantly as dispersivity increases. Dispersion is a deleterious process that can severely limit recovery efficiency.
3. Generally, high formation permeability causes poor recovery efficiencies. When the simulated permeability was increased by a factor of 10, recovery efficiency was reduced by 61.5 percent. This is because simulation of a larger permeability allowed for easier transport of the injected fluid, which resulted in greater stratification and buoyancy flow.
4. When the injection well was represented as open to only part of the aquifer, simulations show little difference as when the well was open to the entire aquifer.
5. For hypothetical conditions studied, porosity and anisotropy variations do not significantly alter recovery efficiencies.

The preliminary radial-flow and solute transport model also was used to examine the effects on recovery efficiency of hypothetical multicycle operations. Simulations consisted of five injection/withdrawal cycles of various duration and varying injection and withdrawal rates. Results of the simulations are:

1. Over the range of variables studied, the recovery efficiency per cycle increases with total number of cycles, provided that each recovery cycle phase ends when the DS concentration of withdrawn water reaches some prescribed value less than that of the more saline formation water. Thus, even though conditions may be such that recovery would be poor on the first cycle, the process should improve on subsequent cycles.
2. Recovery efficiencies increase rapidly during initial cycles and more slowly at later cycles. Recovery efficiencies may approach a maximum value after a number of cycles.
3. For a given operational scheme, recovery efficiencies increase with higher volumes of injected effluent. There is a larger rate of increase of recovery efficiency at small injection/withdrawal volumes than at larger injection/withdrawal volumes.

The operation of a single SSR well appears to be technically feasible under moderately favorable conditions. Model results indicate that recovery efficiencies from about 23 to 37 percent can be achieve for different SSR operational schemes. Five successive injection, storage, and recovery cycles and varying injection and recovery rates can increase the recovery efficiency to about 47 to 62 pecent. The recovery efficiency that will be attained, however, is highly dependent upon local physical and operational conditions. A combination of hydraulic, chemical, and operational parameters that minimize dispersion and buoyancy flow, maximizes recovery efficiency. The parameters that favor optimum recovery efficiencies are low aquifer water density and low to moderate permeabilities. SSR is most promising where native fluid density is low. The smaller the density contrast between resident formation water and injected water the better the recovery efficiency. A high injection rate and a small difference in density between the injected and resident formation waters should yield better results than a low injection rate and a large difference in density. Recoverability improves with successive cycles of injection, storage, and recovery even if initial recovery efficiency is low.

The results presented are preliminary and make up a part of the study in progress. Development of a fully three-dimensional variable density-ground-water flow and solute transport model is presently underway to extend the analysis to multiwell systems for testing of large-scale injection. In a field application of the SSR process, a well field likely will be needed to handle the required inflow rates and wellhead pressures.

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APPENDIX

APPENDIX: LISTING OF MODEL INPUT FILE

A sample input-data listing is provide for the single cycle base simulation of 15 days of injection at 1.0 million gallons per day followed by 15 days of withdrawal at 1.0 million gallons per day. The listing contains 276 lines, of which 147 lines are comments that aid construction of the data file. Critical comments are keyed to input record descriptions of Kipp (1987). The following order generally is observed for data input: (1) fundamental and dimensioning information, (2) spatial geometry and mesh information, (3) fluid properties, (4) porous medium properties, (5) source information, (6) boundary condition information, (7) initial condition information, (8) calculation parameters, and (9) out specifications.

SAMPLE INPUT FILE: INJECT 1 MGAL/D FOR 15 DAYS FOLLOWED BY 15 DAYS

OF WITHDRAWAL AT 1 MGAL/D

```
C.....HST Data-Input Form

C.....UNRELEASE 2.0
C------------------------------------------------------------------------------
C.....Start of the data file
C.....Specification and dimensioning data - READ1
C.1.1 .. TITLE LINE 1
Permeable Zone A simulation for St.Pete--1 Mgal/d injection followed by 1 Mgal/d
C.1.2 .. TITLE LINE 2
withdrawal--3 layers--initial mass fraction zone A = 0.25 (5000 TDS-2375 Cl)
C.1.3 .. RESTRT[T/F],TIMRST
F 0.0
C.1.4 .. HEAT[T/F],SOLUTE[T/F],EEUNIT[T/F],CYLIND[T/F],SCALMF[T/F]
F T T T T
C.1.5 .. TMUNIT[I]
4
C.1.6 .. NX,NY,NZ,NHCN
88,1,26,0
C.1.7 .. NSBC,NFBC,NAIFC,NLBC,NHCBC,NWEL
1 0 0 0 0 1
C.1.8 ..SLMETH[I]
1
C------------------------------------------------------------------------------
C.....Static data - READ2
C.....Coordinate geometry information
C.....   Cylindrical coordinates
C.2.2B.1A .. R(1),R(NR),ARGRID[T/F];(O) - CYLIND [1.4]
1. 2500. F
C.2.2B.1B .. R(I);(O) - CYLIND [1.4] and NOT ARGRID [2.2B.1A]
   1.00   1.14   1.30   1.49   1.70   1.94   2.22   2.53    2.89    3.31
   3.78   4.31   4.92   5.62   6.42   7.33   8.38   9.57   10.93   12.48
  14.25  16.28  18.59  21.23  24.24  27.69  31.62  36.12   41.25   47.11
  53.80  61.44  70.17  80.14  91.52 104.53 119.38 136.34  155.71  177.83
 203.09 231.94 264.90 302.53 350.   400.   450.   500.    550.    600.
 650.   700.   750.   800.   850.   900.   950.  1000.   1050.   1100.
1150.  1200.  1250.  1300.  1350.  1400.  1450.  1500.   1550.   1600.
1650.  1700.  1750.  1800.  1850.  1900.  1950.  2000.   2050.   2100.
2150.  2200.  2250.  2300.  2350.  2400.  2450.  2500.
C.2.2B.2 .. UNIGRZ[T/F];(O) - CYLIND [1.4]
F
C.2.2B.3B .. Z(K);(O) - NOT UNIGRZ [2.2B.3A],CYLIND [1.4]
  0.  50. 100. 130. 150. 160. 170. 180. 190. 200. 210. 220. 230. 240. 250
260. 270. 280. 290. 300. 310. 320. 330. 350. 380. 420.
C------------------------------------------------------------------------------
C.....Fluid property information
C.2.4.1 .. BP
3.03E-6
C.2.4.2 .. P0,T0,W0,DENF0
14.7 75.0 0 62.241
C.2.4.3 .. W1,DENF1;(O) - SOLUTE [1.4]
0.020 63.1772
C.2.5.1 .. VISFAC
-0.8904
C------------------------------------------------------------------------------
C.....Reference condition information
C.2.6.1 .. PAATM
14.7
C.2.6.2 .. P0H,T0H
0,75.0
C------------------------------------------------------------------------------
```

```
C.....Solute information
C.2.8 .. DM,DECLAM;(O) - SOLUTE [1.4]
9.30E-5,0
C-----------------------------------------------------------------------------
C.....Porous media zone information
C.2.9.1 .. IPMZ,X1Z(IPMZ),X2Z(IPMZ),Y1Z(IPMZ),Y2Z(IPMZ),Z1Z(IPMZ),Z2Z(IPMZ)
1 1 2500. 1 1 0. 150.
2 1 2500. 1 1 150. 330.
3 1 2500  1 1 330. 420.
END
C-----------------------------------------------------------------------------
C.....Porous media property information
C.2.10.1 .. KXX(IPMZ),KYY(IPMZ),KZZ(IPMZ),IPMZ=1 to NPMZ [1.7]
3.877E-12,,3.877E-12
6.475E-10,,6.475E-10
3.102E-15,,3.102E-15
C.2.10.2 .. POROS(IPMZ),IPMZ=1 to NPMZ [1.7]
.3 .3 .3
C.2.10.3 .. ABPM(IPMZ),IPMZ=1 to NPMZ [1.7]
6.2E-6 6.2E-6 6.2E-6
C-----------------------------------------------------------------------------
C.....Porous media solute and thermal dispersion information
C.2.12 .. ALPHL(IPMZ),ALPHT(IPMZ),IPMZ=1 to NPMZ [1.7];(O) - SOLUTE [1.4]
C..         and/or HEAT [1.4]
12.5 2.5
12.5 2.5
12.5 2.5
C-----------------------------------------------------------------------------
C.....Porous media solute property information
C.2.13 .. DBKD(IPMZ),IPMZ=1 to NPMZ [1.7];(O) - SOLUTE [1.4]
3*0.0
C-----------------------------------------------------------------------------
C.....Source-sink well information
C.2.14.1 .. IWEL,XW,YW,ZBW,ZTW,WBOD,WQMETH[I];(O) - NWEL [1.6] >0
C.2.14.2 .. WCF(L);L = 1 to NZ (EXCLUSIVE) by ELEMENT
C.2.14.3 .. WSF(L);L = 1 to NZ (EXCLUSIVE) by ELEMENT
1 1 1 150. 330. 2. 11
0,0,0,0,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,0,0,0
25*0
END
C-----------------------------------------------------------------------------
C.....Boundary condition information
C-----------------------------------------------------------------------------
C.....     Specified value b.c.
C.2.15 .. IBC by x,y,z range {0.1-0.3} with no IMOD parameter;(O) -
C..         NSBC [1.6] > 0
1. 2500. 1. 1. 420. 420.
101
1. 2500. 1. 1. 0. 0.
101
2500. 2500. 1 1 50. 150.
101
2500. 2500. 1 1 150. 330.
101
2500. 2500. 1 1 330. 380.
101
END
C-----------------------------------------------------------------------------
C.....Free surface b.c.
C.2.20 .. FRESUR[T/F],PRTCCM[T/F]
F F
C-----------------------------------------------------------------------------
C.....Initial condition information
C.2.21.1 .. ICHYDP,ICTPRO,ICCPRO; all [T/F]
T F F
C.2.21.3A .. ZPINIT,PINIT;(O) - ICHYDP [2.21.1] and NOT ICHWT [2.21.2]
```

```
450. 0.
C.2.21.6B .. C by x,y,z range {0.1-0.3};(O) - SOLUTE [1.4] and NOT ICCPRO
C..          [2.21.1]
1 2500. 1 1 0. 130.
1 1
1 2500. 1 1 150. 320.
0.25 1
1 2500. 1 1 330. 420.
0.0250 1
END
C-------------------------------------------------------------------------------
C.....Calculation information
C.2.22.1 .. FDSMTH,FDTMTH
0 1.
C.2.22.2 .. TOLDEN{.001},MAXITN{5}
.1 10
C.2.22.3 .. EPSFS;(O) - FRESUR [2.20]
C-------------------------------------------------------------------------------
C.....Output information
C.2.23.1 .. PRTPMP,PRTFP,PRTIC,PRTBC,PRTSLM,PRTWEL; all [T/F]
6*T
C.2.23.2 .. IPRPTC,PRTDV[T/F];(O) - PRTIC [2.23.1]
201 T
C.2.23.3 .. ORENPR[I];(O) - NOT CYLIND [1.4]
C.2.23.4 .. PLTZON[T/F];(O) - PRTPMP [2.23.1]
F
C.2.23.5 .. PLTTEM[T/F]
F
C-------------------------------------------------------------------------------
C..... TRANSIENT DATA - READ3
C.3.1 .. THRU[T/F]
F
C-------------------------------------------------------------------------------
C.....Source-sink well information
C.3.2.1 .. RDWTD[T/F];(O) - NWEL [1.6] > 0
T
C.3.2.2 .. IWEL,QWV,PWSUR,PWKT,TWSRKT,CWKT;(O) - RDWTD [3.2.1]
1 133690. 0 51.87 75.0 0.035
END
C-------------------------------------------------------------------------------
C.....Boundary condition information
C-------------------------------------------------------------------------------
C.....     Specified value b.c.
C.3.3.1 .. RDSPBC,RDSTBC,RDSCBC; all [T/F];(O) - NSBC [1.6] > 0
T F T
C.3.3.2 .. PNP B.C. by x,y,z range {0.1-0.3};(O) - RDSPBC [3.3.1]
1 2500. 1 1 420. 420.
12.967 1
1 2500. 1 1 0. 0.
195.719 1
2500. 2500. 1 1 50. 380.
3 5
50. 173.702 380. 30.256
END
C..          SOLUTE [1.4] ALWAYS NEED THIS IF SPEC PRESS BOUNDARY
END
C.3.3.6 .. CNP B.C. by x,y,z range {0.1-0.3};(O) - RDSCBC [3.3.1] and
C..          SOLUTE [1.4]
1 2500. 1 1 420. 420.
0.0250 1
1 2500. 1 1 0. 0.
1 1
2500. 2500. 1 1 50. 50.
1 1
2500. 2500. 1 1 100. 100.
```

```
1 1
2500. 2500. 1 1 130. 130.
1 1
2500. 2500. 1 1 150. 150.
0.25 1
2500. 2500. 1 1 150. 320.
0.25 1
2500. 2500. 1 1 330. 380.
0.0250 1
END
C-----------------------------------------------------------------------------
C.....Calculation information
C.3.7.1 .. RDCALC[T/F]
T
C.3.7.2 .. AUTOTS[T/F];(O) - RDCALC [3.7.1]
f
C.3.7.3.A .. DELTIM;(O) - RDCALC [3.7.1] and NOT AUTOTS [3.7.2]
0.5
C.3.7.3.B .. DPTAS{5E4},DTTAS{5.},DCTAS{.25},DTIMMN{1.E4},DTIMMX{1.E7};
C..          (O) - RDCALC [3.7.1] and AUTOTS [3.7.2]
C.3.7.4 .. TIMCHG
15.
C-----------------------------------------------------------------------------
C.....Output information
C.3.8.1 .. PRISLM,PRIKD,PRIPTC,PRIDV,PRIVEL,PRIGFB,PRIBCF,PRIWEL; all [I]
0 0 -15. 0 0 0 0 -15.
C.3.8.2 .. IPRPTC;(O) - IF PRIPTC [3.8.1] NOT = 0
201
C.3.8.3 .. CHKPTD[T/F],PRICPD,SAVLDO[T/F]
F /
C-----------------------------------------------------------------------------
C.....Contour and vector map information
C.3.9.1 .. CNTMAP[T/F],VECMAP[T/F],PRIMAP[I]
T T -15.0
C-----------------------------------------------------------------------------
C.....END OF FIRST SET OF TRANSIENT INFORMATION
C.....TRANSIENT DATA -READ3
C.....SECOND STAGE WITHDRAW 1MGAL/D FOR 15 DAYS........................
C-----------------------------------------------------------------------------
C.3.1 .. THRU[T/F]
F
C-----------------------------------------------------------------------------
C.....Source-sink well information
C.3.2.1 .. RDWTD[T/F];(O) - NWEL [1.6] > 0
T
C.3.2.2 .. IWEL,QWV,PWSUR,PWKT,TWSRKT,CWKT;(O) - RDWTD [3.2.1]
1 -133690. 0 51.87 75.0 0.035
END
C-----------------------------------------------------------------------------
C.....Boundary condition information
C-----------------------------------------------------------------------------
C.....     Specified value b.c.
C.3.3.1 .. RDSPBC,RDSTBC,RDSCBC; all [T/F];(O) - NSBC [1.6] > 0
T F T
C-----------------------------------------------------------------------------
C.....Calculation information
C.3.7.1 .. RDCALC[T/F]
T
C.3.7.2 .. AUTOTS[T/F];(O) - RDCALC [3.7.1]
f
C.3.7.3.A .. DELTIM;(O) - RDCALC [3.7.1] and NOT AUTOTS [3.7.2]
0.25
C.3.7.4 .. TIMCHG
30.
C-----------------------------------------------------------------------------
C.....Output information
```

```
C.3.8.1 .. PRISLM,PRIKD,PRIPTC,PRIDV,PRIVEL,PRIGFB,PRIBCF,PRIWEL; all [I]
0 0 1 0 0 0 0 1
C.3.8.2 .. IPRPTC;(O) - IF PRIPTC [3.8.1] NOT = 0
201
C.3.8.3 .. CHKPTD[T/F],PRICPD,SAVLDO[T/F]
F /
C-------------------------------------------------------------------------------
C.....Contour and vector map information
C.3.9.1 .. CNTMAP[T/F],VECMAP[T/F],PRIMAP[I]
T T -30.
C-------------------------------------------------------------------------------
C.....End of second set of transient information
C.....End of simulation line follows, THRU=.TRUE.
C.3.99.1 .. THRU
T
C......End of the data file
```