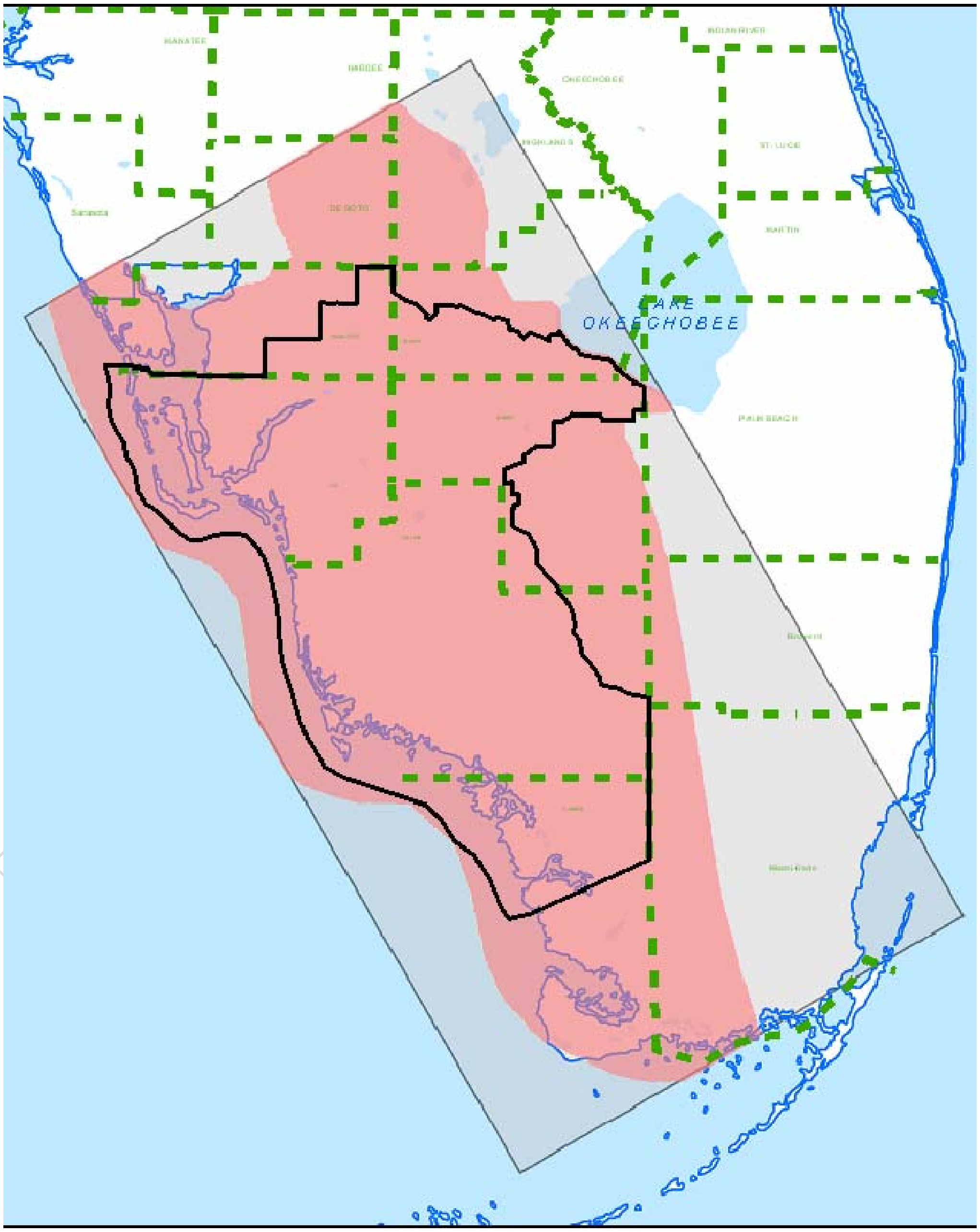
LOWER WEST COAST FLORIDAN AQUIFER MODEL



FAU
FLORIDA ATLANTIC UNIVERSITY

SOUTH FLORIDA WATER MANAGEMENT DISTRICT

A Density-Dependent Groundwater Flow Model of the Lower West Coast Floridan Aquifer System

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Jorge Restrepo
David Garces
Angela Montoya

Prepared by
Florida Atlantic University
Department of Geosciences

In Association With
South Florida Water Management District
Water Supply Department
Model Application Section

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Tom Corcoran and Tobin Hindle

Contributors:
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Executive Summary

The Lower West Coast Floridan Aquifer System (LWCFAS) Model is a three-dimensional, density-dependent groundwater flow and transport model that has been developed as a predictive and interpretive tool in association with the South Florida Water Management District (SFWMD). This model can analyze different water management scenarios for water supply plans and ecosystem restoration efforts on a regional basis. The model was developed using a modified version of the USGS three-dimensional finite-difference flow code, MODFLOW-2000, known as SEAWAT-2000. The source code for SEAWAT-2000 was developed by combining MODFLOW and MT3DMS into a single program that solves both coupled-flow and solute-transport equations.

Two versions of the LWCFAS Model are available for the study area. The first model domain is discretized into 72 rows and 37 columns, with a uniform cell-size of 12,000 feet by 12,000 feet. It includes twelve, vertical layers representing lithologic zones within the surficial, intermediate, and Floridan aquifer systems. The second model domain is discretized into 287 rows and 150 columns, with a uniform cell-size of 3,000 feet by 3,000 feet, and has a vertical discretization that mirrors the first model.

Both models provide a valuable insight toward understanding the mechanisms and processes that drive this system, including the variation in aqueous salinity. The model presented herein is based on raw data obtained by the SFWMD, SWFWMD, USGS, NOAA and the Center of Geosciences at Florida Atlantic University (CG-FAU). The main advantage of both models, besides incorporating the high degree of aquifer heterogeneity, is the ability of the models to simulate the chloride distribution within the system. The model calibration period was from January 1997 to December 2001. The first model with a uniform cell-size of 12,000 feet by 12,000 feet was used for the pre-development, quasi-steady-state calibration. From this calibrated model, the second model was developed with a uniform cell size of 3,000 feet by 3,000 feet. This finer resolution model produced acceptable results given limited available data.

In the end, a model is any device that represents an approximation of a field situation. As with all models, this model is an approximation of reality and should be improved and refined continuously in the future as the knowledge-base expands. Again, as with most model applications, the utmost value of the model is not its predictive abilities, but the deeper conceptual understanding that is gained during the process of continual use and improvement. It is truest in the current model where the lack of measured data is considerable.

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Acronyms and Abbreviations

ac-ft	acre-feet
aerial photo quad	topographical quadrant map overlain on an aerial photograph
ADV	Advection package
AGR	agriculture (water use category)
APT	aquifer performance test
ASCII	American Standard Code for Information Interchange
ASR	aquifer storage and recovery
AWS	alternative water supply
AWWA	American Water Works Association
Aq1b	Aquifer layer 1 bottom
Aq2t	Aquifer layer 2 top
Aq3b	Aquifer layer 3 bottom
Aq3t	Aquifer layer 3 top
Aq4b	Aquifer layer 4 bottom
Aq4t	Aquifer layer 4 top
BAS	Basic package
BCF	Block Centered Flow package
bls	below land surface
BP	Before Present
BTN	Basic Transport package
BZ	Boulder zone
CCMP	Comprehensive Conservation and Management Plan
CERP	Comprehensive Everglades Restoration Plan
cfs	cubic feet per second
CG-FAU	Center of Geosciences at Florida Atlantic University
CHD	Constant Head package
cm	centimeter
CPU	Central Processing Unit

CUP	consumptive use permitting
CWA	Clean Water Act
CWMP	Caloosahatchee Water Management Plan
DBHydro	SFWMD's corporate environmental database
DBKey	database key used in DBHydro database
DERM	Department of Environmental Resource Management
DIS	Discretization package
District	South Florida Water Management Distric
DIV	Diversion package
DOM	Domestic (water use category)
DOQ	digital ortho quadrangle (electronic aerial photography)
DRN	Drain package
DSP	Dispersion package
DWMP	District Water Management Plan
DWSA	Districtwide Water Supply Assessment
ENP	Everglades National Park
ERP	environmental resource permitting
ET	evapotranspiration
FAS	Floridan aquifer system
FAU	Florida Atlantic University
FDEP	Florida Department of Environmental Protection
FGS	Florida Geological Survey
FORTRAN	Formula Translation Model
F.S.	Florida Statutes
FY	fiscal year
GCG	Generalized Conjugate Gradient Solution package
GHB	General Head Boundary package of MODFLOW
GHz	Gigahertz
GIS	geographic information system
GLO	Global
GLO1	Global Process

GOL	golf course irrigation (water use category)
GPCD or gpcd	gallons per capita per day
GPD or gpd	gallons per day
GPD/ft	gallons per day per unit foot
GPM or gpm	gallons per minute
GWF	Ground-Water Flow
GWF1	Ground-Water Flow Process
HAEDC	Geological Survey High-Accuracy Elevation Data Collection
HARN	High Accuracy Reference Network
HBXY	Boundary Head Interpolation package
HORIZ	Horizontal
IAS	Intermediate aquifer system
IC	intermediate confining unit
IMT	Integrated MT3DMS Transport
IMT1	Integrated MT3DMS Process
IND	industrial (water use category)
IRR	irrigation (water use category)
km	kilometers
Kx	horizontal hydraulic conductivity
Kz	vertical hydraulic conductivity
LAN	landscape irrigation (water use category)
LEC	Lower East Coast
LF1	first permeable zone of the Lower Floridan aquifer
LFA	Lower Floridan aquifer
LFbot	Lower Floridan bottom
LFC1	Lower Floridan aquifer confining unit 1
LFtop	Lower Floridan top
LHA	Lower Hawthorn aquifer
LHPZ	Lower Hawthorn producing zone
LIV	Livestock (water use category)
LPF	Layer Property Flow package

LTA	Lower Tamiami aquifer
LWC	Lower West Coast
LWCFAS	Lower West Coast Florida aquifer system
m	meters
MAE	mean absolute error
Max	maximum
MC1	Upper Middle confining unit
MC2	Lower Middle confining unit
MCtop	Middle confining unit top
MCU	Middle confining unit
MF	Middle Floridan aquifer
MFbot	Middle Floridan bottom
MFtop	Middle Floridan top
mg/L	milligrams per liter
MGD or mgd	million gallons per day
mg/L	milligrams per liter
MGY or mgy	million gallons per year
MHHW	Mean Higher High Water
Min	minimum
MLLW	Mean Lower Low Water
mm	millimeters
MODFLOW	A U.S. Geological Survey MODular 3-dimensional finite-difference groundwater FLOW model
MSL or msl	mean sea level
MT3DMS	A Modular 3-D Multispecies Transport Model
NA	not applicable or not available
NAVD88	North American Vertical Datum of 1988
NGVD29	National Geodetic Vertical Datum of 1929
NGS	National Geodetic Survey
NOAA	National Ocean and Atmospheric Administration
NOS	National Ocean Service

NPS	National Park System
NRCS	Natural Resources Conservation Service
OBS	Observation
OBS1	Observation Process
OBSG	Observation plotting program
OTH	Other (water use category)
PBC	Palm Beach County
PCG	Pre-conjugate Gradient- Solution package
PDE	partial differential equation
PEST	Parameter ESTimation (an automated parameter optimization software)
PP	Pilot Points
ppm	parts per million
PR	predicted water levels
psi	pounds per square inch
PWS	public water supply
QA/QC	quality assurance and quality control
R2	correlation coefficient
RAM	Random Access Memory
RDF	Reinjection Drain Flow package
RECOVER	Restoration, Coordination, and Verification
Restudy	Central and Southern Florida Project Comprehensive Review Study
RIV	River package
RMS	Root Mean Square
RO	reverse osmosis
SAS	surficial aquifer system
SEAWAT-2000	U.S. Geological Survey Modular Ground-Water Model for simulating three-dimensional, variable-density, groundwater flow
SFWMD	South Florida Water Management District
SFWMM	South Florida Water Management Model
SIP	Strongly Implicit Procedure

SJRWMD	St. Johns River Water Management District
SOW	Statement of Work
SR	State Road
SRC	Source (water use category)
SS	Specific Storage
SSM	Source-Sink Mixing package
STA	Sandstone Aquifer
STORA	Storativity
SVD-ASSIST	truncated singular value decomposition (A program in PEST)
SWFWMD	South West Florida Water Management District
TDS	Total Dissolved Solids
Topo	topography – ground surface
topo quad map	topographical quadrant map
Trans	Transmissivity
UFA	Upper Floridan aquifer
UFtop	Upper Floridan top
UGEN	Utility Generation package
UIC	underground injection control
ULFA	upper part of the Lower Floridan aquifer
U.S.	United States
USACE	United States Army Corps of Engineers
USDA	United States Department of Agriculture
USDOI	United States Department of Interior
USDW	Underground Sources of Drinking Water
USEPA	United States Environmental Protection Agency
USGS	United States Geological Survey
VDF	Variable-Density Flow
VDF1	Variable-Density Flow Process
VERT	Vertical
WCA	water conservation area
WEL	MODFLOW well package

CHAPTER 1
INTRODUCTION

BACKGROUND

The study area focuses on the Lower West Coast (LWC) Planning Area, which covers roughly 4,255 square miles and consists of freshwater lakes, wetlands and estuaries, uplands, agricultural and urban areas, and coastal ecosystems lying within a highly managed system of canals, operational structures, levees, and retention ponds (see **Figure 1-1**). Increased population growth in this area continues to drive water demands higher. The new water use demands must be balanced with the water needs of the environment. Experts are predicting that the LWC Planning Area will experience substantial growth between the year 2005 and the year 2025. Population is expected to increase from the roughly 910,000 in 2005 to about 1.6 million in 2025 (U.S. Bureau of the Census 2001). Most of the population growth is expected in Lee and Collier counties. This growth will create additional demands for both potable and irrigation water. Urban water demand (municipal, domestic self-supply, recreational and commercial) in the planning area will increase by approximately 114 MGD due to the population surge. Water demand associated with new power generation facilities proposed for the planning area will increase by about 66 MGD. Agricultural acreage under cultivation in the LWC Planning Area is projected to increase by 13,400 acres, in part reflecting a shift in agricultural operations from Lee and Collier counties to Glades and Hendry counties, with the latter move requiring an additional estimated 17 MGD worth of supply (SFWMD 2006).

The surficial and intermediate aquifer systems and the Caloosahatchee River have traditionally been the primary sources of water within the LWC Planning Area. The physical limitations of these sources, however, along with the threat of saltwater intrusion and the need to protect valuable natural areas limit their ability to provide significant additional water to this rapidly growing area. These conditions necessitate the development of alternative sources of water to curb the pressures exerted on present water supplies and guarantee the long-term survival of the region's natural systems and water resources. One such alternative is the development of the Floridan aquifer system (FAS).

The FAS underlies the entire state of Florida and parts of Georgia, South Carolina, and Alabama, and is used as the principal source of water in north and central Florida, but until recent years, has been only lightly used within the LWC. In striving toward the goal of investigating and identifying potential alternative water sources (SFWMD 2006), the South Florida Water Management District (SFWMD) initiated the development of the Lower West Coast Floridan Aquifer System (LWCFAS) Model.

This model will be used to support: ongoing water supply management and ecosystem restoration efforts, Lower West Coast (LWC) Water Supply Plan (Section 373.0361, F.S.) development, evaluation of regional water resource and water supply development projects, and most fundamentally, the understanding of the processes and hydrogeologic framework that govern the movement of water within the Floridan aquifer system.

PURPOSE AND SCOPE

Saltwater intrusion is a perennial problem in coastal aquifers. Understanding and controlling it is complicated when the aquifer extends offshore beneath the Gulf of Mexico (Gulf) floor, as is the case in the FAS. Barring anthropogenic interventions, the brackish waters of the Upper Floridan aquifer (UFA), which is the primary target for alternative supplies, continue to flow outward past the coastline, eventually ending in Gulf waters somewhere offshore. This outward flow continues if a sufficiently high hydraulic head exists to maintain a static saltwater/freshwater interface offshore. As anthropogenic development of the aquifer occurs, groundwater is diverted into pumping wells. The hydraulic head declines and the saltwater/freshwater interface migrates landward until a new, more stable salinity distribution is achieved. This process may occur across a geologic time-scale that we find imperceptible, or, if the hydrogeologic conditions are right, the movement may be much more rapid.

Current water quality in the FAS ranges from brackish to saline within the project area; salinity increases with depth and proximity to the coast. The saline nature of the water quality has restricted its use to public water supplies, having the ability to desalinate the water. Increasing numbers of urban utilities within the LWC Planning Area have begun to use the FAS in this manner. There is significant uncertainty, however, about the long-term water quality impacts of these sustained withdrawals. The need to evaluate this uncertainty for existing users and project changes in flow and quality from new consumptive uses necessitates a predictive density-dependent flow and transport model. Florida Atlantic University (FAU), in conjunction with the SFWMD, undertook the development of such a model for the intermediate and Floridan aquifer systems within the LWC Planning Area.

This report documents the development of the three-dimensional, numerical model, which simulates transient groundwater flow in the LWC Planning Area. This technical document helps familiarize engineers, hydrogeologists, project stakeholders, and the general public with the model and its potential applications. However, it is not intended as an official user's manual of the model's many applications.

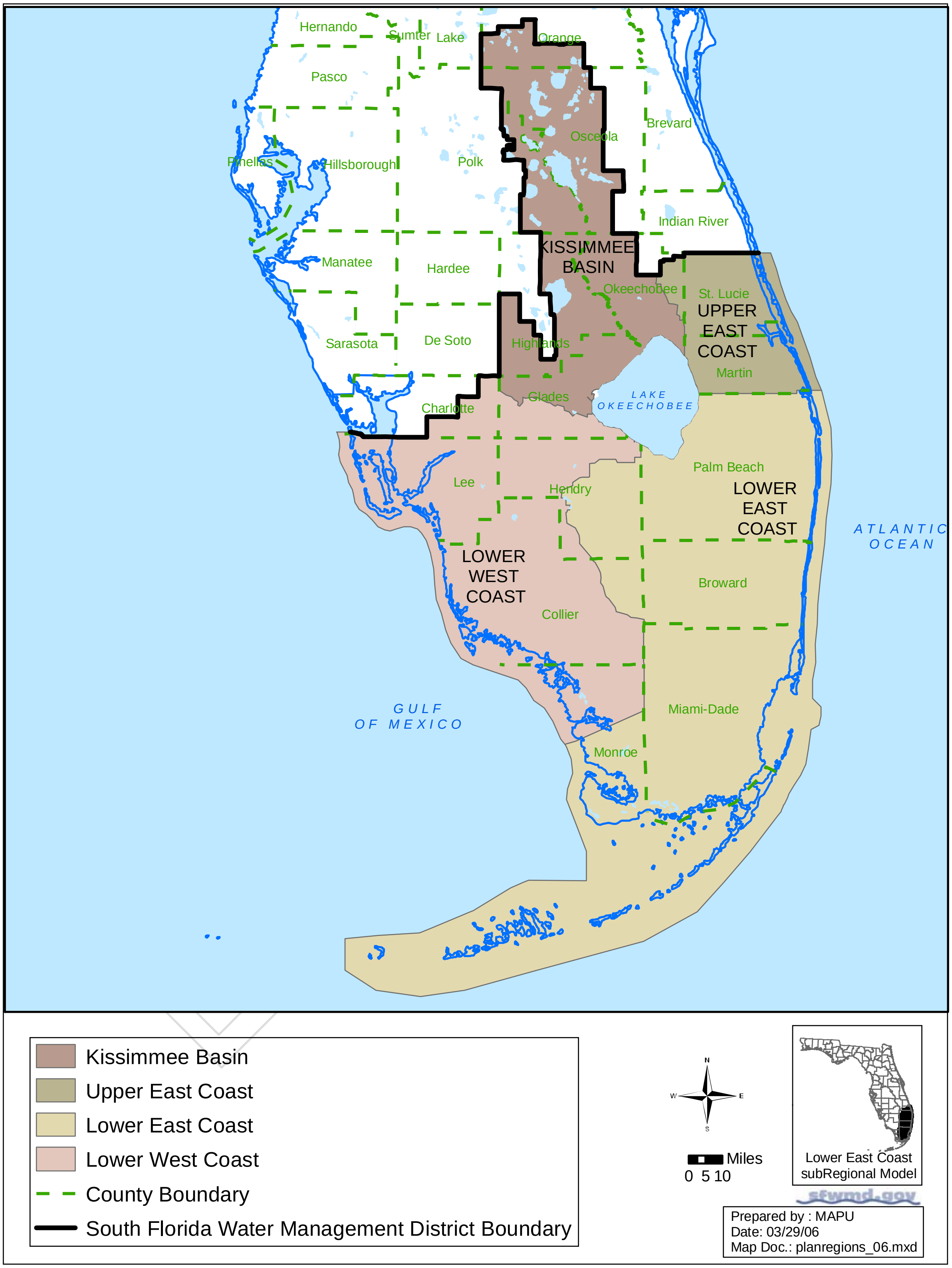

Figure 1-1. Boundaries for the South Florida Water Management District Planning Areas.

The scope of this document covers the development of the model in its entirety. **Chapter 1** has introduced the purpose and scope of this study, while referencing previous modeling studies that have supported SFWMD goals. **Chapter 2** discusses the development of the conceptual model and how available data is collected and assembled to define the hydrogeologic system. **Chapter 3** reviews code selection and model design, which are two important aspects of simulating flow. **Chapter 4** describes the process of model calibration and the results of sensitivity analysis. Finally, **Chapter 5** presents the conclusions and recommendations with respect to model capabilities, limitations, and future improvements.

PREVIOUS STUDIES

A comprehensive review of all previous research pertaining to the FAS in southwestern Florida is beyond the scope of this project. Numerous authors representing public agencies, private consultants, and universities have contributed to the body of knowledge of the FAS within the study area. This discussion will focus on those reports most pertinent to this modeling effort.

Reese (2000), in his USGS report, "Hydrogeology and the Distribution of Salinity in the Floridan Aquifer System," studied the hydrogeological framework of the FAS and related the distribution of salinity in the aquifer system to that same framework. His research showed that the FAS could well be considered a valuable supplemental source of public water supply in southwestern Florida even though it contains only brackish water. There are large areas in the FAS of relatively low salinity in the Hawthorn Group that could be used as a potential source of water (Reese 2000). Additionally, Reese and Richardson (2004, in press) integrated past research on the FAS (from Orlando to Key West) to form a single comprehensive view of the hydrostratigraphy and hydraulic properties of the FAS, which is largely used in the development of this model.

Sepulveda (2002) developed a MODFLOW-96 groundwater flow model for both the intermediate aquifer system (IAS) and FAS in peninsular Florida. He sought to (1) test and refine the conceptual understanding of the regional groundwater flow system; (2) develop a database to support subregional groundwater flow modeling; and (3) evaluate the effect of projected 2020 groundwater withdrawals on groundwater levels (Sepulveda 2002).

Shoemaker and Edwards (2003) conducted their study to examine the potential for saltwater intrusion in the Lower Tamiami aquifer beneath Bonita Springs in southwestern Florida. They examined potential mechanisms of saltwater intrusion which included (1) lateral inland movement of the freshwater-saltwater interface from the southwestern coast of Florida; (2) upward leakage from deeper saline water-bearing zones through natural upwelling and upconing; (3) downward leakage of salt water from surface water channels; and (4) movement of unflushed pockets of relict seawater into the Lower Tamiami aquifer (Shoemaker and Edwards 2003).

Bennett (2001) carried out investigations of the FAS at the L-2 Canal Site in Hendry County. His investigations included documentation of the hydrogeology, water quality, productive capacity and long-term, potentiometric head data of three, Floridan aquifer test wells. Results from Bennett's (2001) technical publication indicated limited production capacity in the UFA in this area, noting chloride and total dissolved solids (TDS) in the water exceeded potable drinking water standards. Bennett (2002, 2003) also investigated the hydrogeology of the FAS at sites in Collier and northwest Hendry counties. Results at these sites showed moderate to good production capacity in the UFA. Chloride and TDS in the UFA again exceeded potable drinking water standards at the sites therein.

HydroGeoLogic Inc. (2002) developed a density-dependent flow and transport model for the southern water use caution area, north of the study area. Their model encompassed all of Tampa Bay and the Lake Wales Ridge, focusing on the Upper Floridan aquifer. Results from the HydroGeoLogic, Inc. model (2002) showed that the major threat to groundwater quality within the study area was saltwater intrusion. Generally speaking, water quality was good in all aquifers above the Middle confining unit separating the Upper and Lower Floridan aquifers. Conversely, the water quality decreased (and salinity increased with depth) below the Middle confining unit.

CHAPTER 2
MODEL CONCEPTUALIZATION

STUDY AREA

The study area is located in southwestern Florida. Initially it included Lee, Hendry, Collier, Glades and Charlotte counties, but it was extended for modeling purposes to include all or part of Highlands, Hardee, De Soto, Palm Beach, Broward, Monroe and Miami-Dade counties. The active zone of the model, however, involves only all or part of Charlotte, Glades, Lee, Hendry, Collier, Monroe and Miami-Dade counties (**Figure 2-1**). Surface water and groundwater boundaries in southwest Florida are used to detail the study area. Specifically, the limits of the study area coincides with a groundwater divide of the Floridan aquifer system, while the Gulf of Mexico, 60,000 feet offshore, forms the western limit. The northern limit is the area surrounding the Caloosahatchee River, and the southern area is defined by the tip of Florida Bay (**Figure 2-1**). In the vertical direction, the model extends from land surface to the intermediate and Floridan aquifer systems within the Lower West Coast Planning Region.

CLIMATE

The climate of the LWCFAS Model study area is very similar to the climate of the rest of Florida, which is tropical to subtropical. It is marked by a distinctive wet season from May to October and a dry season from November to April. Average annual rainfall is approximately 53 inches with 75 percent falling during the wet season. Close proximity to the Gulf of Mexico serves to moderate the temperature in the study area. Temperatures (in Fahrenheit) rarely exceed the mid 90s during summer months and rarely fall below the high 50s during winter months. Average annual rainfall is approximately 53 inches with 75 percent falling during the wet season.

TOPOGRAPHY AND SURFACE WATER CHARACTERISTICS

The surface elevation in the study area is typically less than 25 feet above sea level. Topographic values were obtained from a combination of the following sources: U.S. Geological Survey High-Accuracy Elevation Data Collection (HAEDC) and 24K quad points and SFWMD/TRT SUPERTOPO directory. These were used to define the top of the surficial aquifer system (SAS). Surface water characteristics are used to define water levels in the SAS. Surface water sources within the LWCFAS Model domain include several canals, a large wetland ecosystem (Everglades), rivers and their tributaries, lakes, and coastal estuaries, including the Gulf of Mexico.

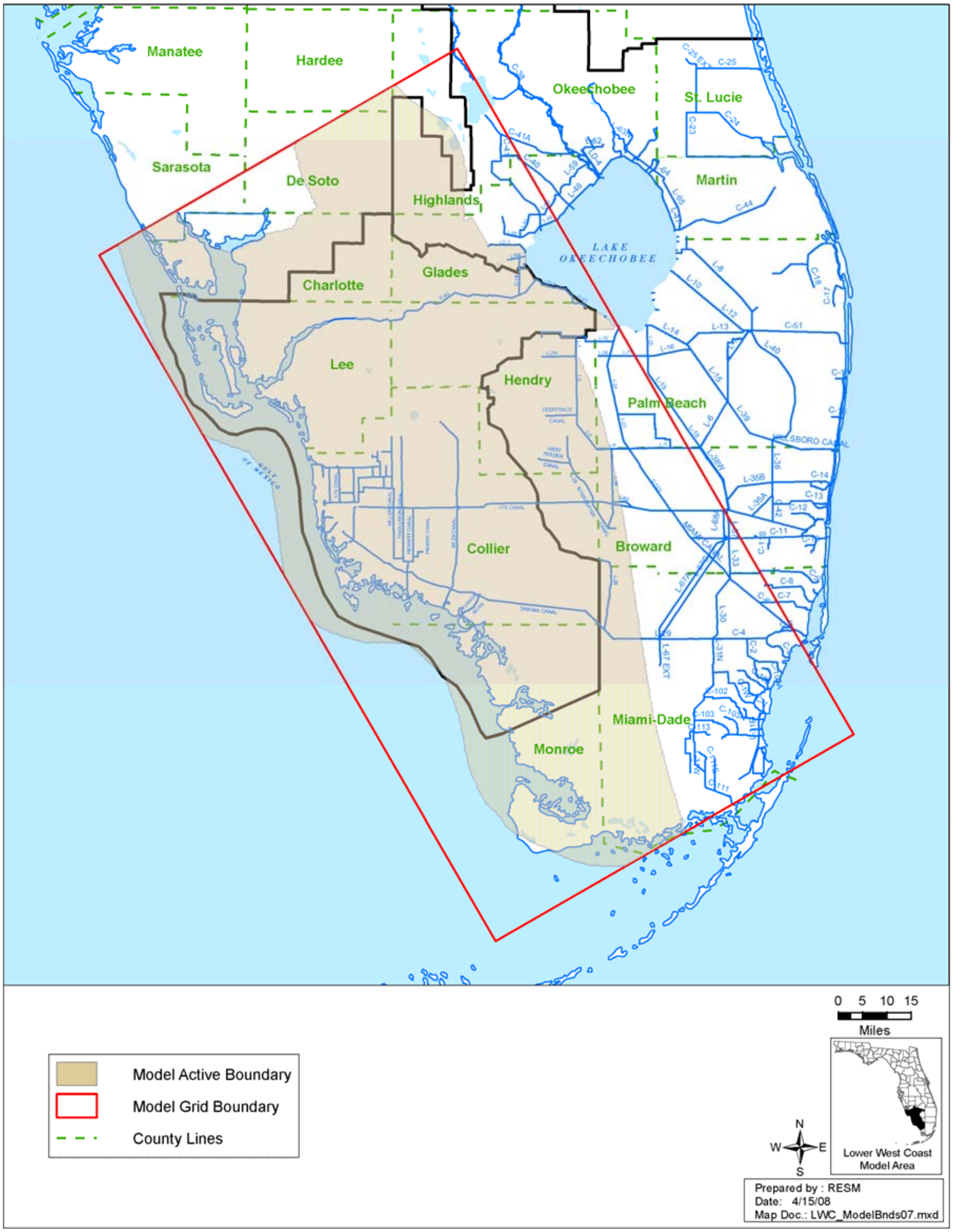

Figure 2-1. General view of the study area.

HYDROGEOLOGY OF SOUTHWESTERN FLORIDA

The basement complex of south Florida is composed of rhyolites and basalts. These rocks are believed to have formed in southwest Florida near the vicinity of an early Mesozoic Era triple junction or hot spot (Heatherington and Mueller 1997). This triple junction is believed to be associated with the breakup of Pangaea. During the late Jurassic and Early Cretaceous, a shallow water limestone began to develop over the volcanic basement complex. These deposits covered a wide area resulting in a "mega-platform" extending from the western edge of the modern Florida Plateau, eastward across the straits of Florida to the Bahama escarpment (Leg 101 Scientific Party 1988). The carbonate platform also appears to have extended southward to the northern coast of Cuba (Denny et al. 1994). This platform became submerged and began to break apart in a stepwise fashion during the mid- to late- Cretaceous, creating the Florida Straits and separating the Florida Plateau from the Bahamas (Leg 101 Scientific Party 1988). The total thickness of these Mesozoic carbonate sediments may exceed 5,000 feet in southwest Florida, specifically in Collier County.

The Peninsular Florida is the emergent (subaerial) portion of the Florida Plateau. Generalized and schematized submarine topography of the continental shelf and the Florida Peninsula (from Meyer 1989 and the SFWMD GIS database) are depicted in **Figure 2-2**, which shows a gradual decline in elevation toward the West Florida Slope. The Florida Plateau is underlain by a sequence of aquifers and confining to semi-confining units that range in age from Paleocene to Pliocene, as shown in **Figure 2-3**. **Figure 2-4** displays the salinity regimes of the saline Lower Floridan aquifer and the brackish Upper Floridan aquifer. This figure also shows the vertical circulation, which occurs through fractures and solution features. The location of section A-A' (from **Figure 2-2**) is depicted in **Figure 2-4.** Note that in **Figure 2-4**, Meyer's (1989) nomenclature is different from terms used by Scott (1988) and Reese and Richardson (2007 in press) to describe what is known presently as the Hawthorn Group, which includes the Peace River and Arcadia Formations. The movement of ground water from inland areas to the ocean and vice versa occurs principally through the carbonate rocks (Meyer 1989).

Lithology and Stratigraphy

The principal water-bearing units in south Florida are generally of Cenozoic age. In south Florida, Cenozoic-age deposits may reach a depth of about 5,500 feet NGVD in the southern portion of the study area (Applin and Applin 1944). **Figure 2-5** shows a geologic map of south Florida (Scott et al. 2001), while the lithostratigraphy is displayed in **Figure 2-**3**.** The primary Cenozoic stratigraphic units in the study area include, from oldest to youngest, the Cedar Keys Formation, Oldsmar Formation, Avon Park Formation, Ocala Limestone, Suwannee Limestone, Hawthorn Group, the Tamiami Formation, and various Pleistocene/Holocene sediments.

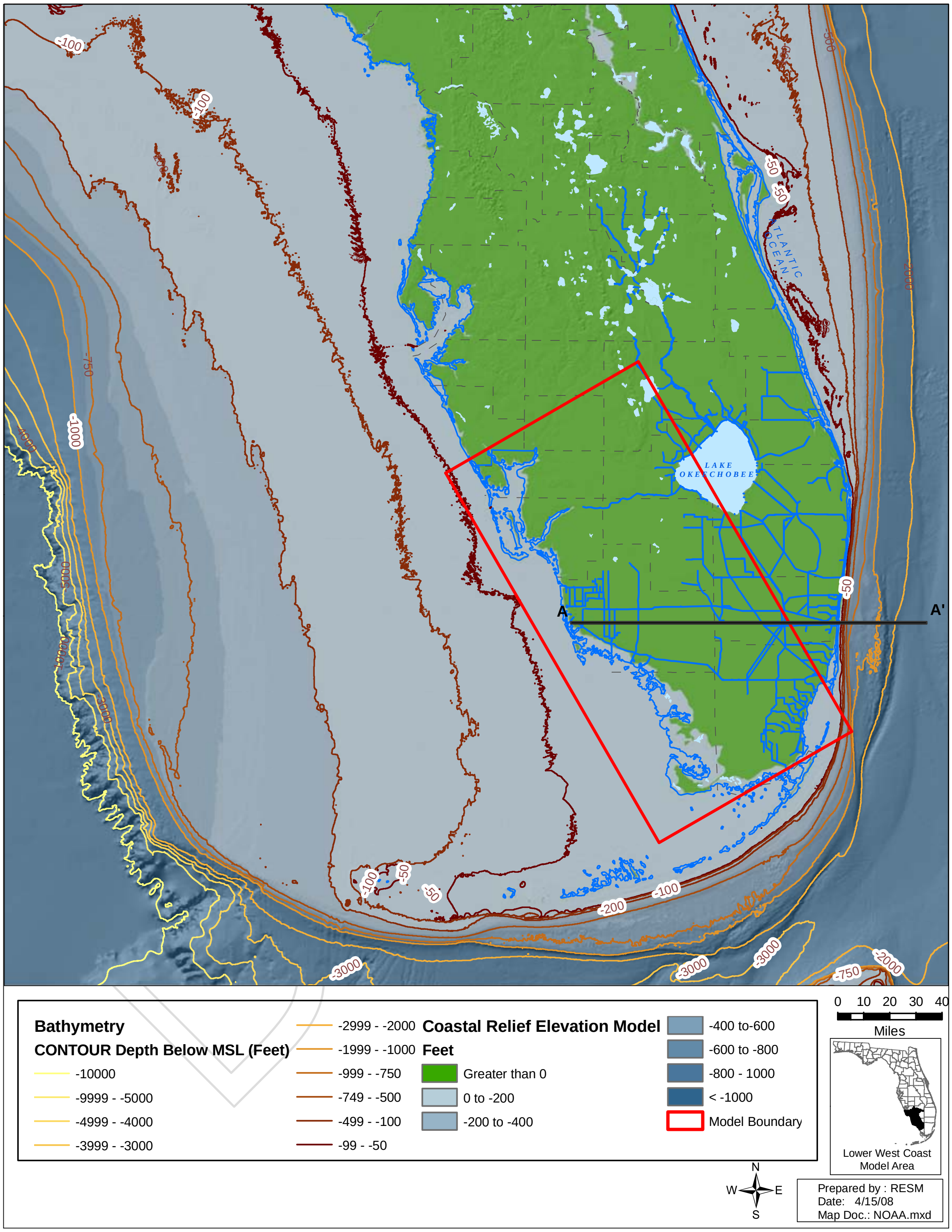

Figure 2-2. South Florida Peninsula with the submarine topography.

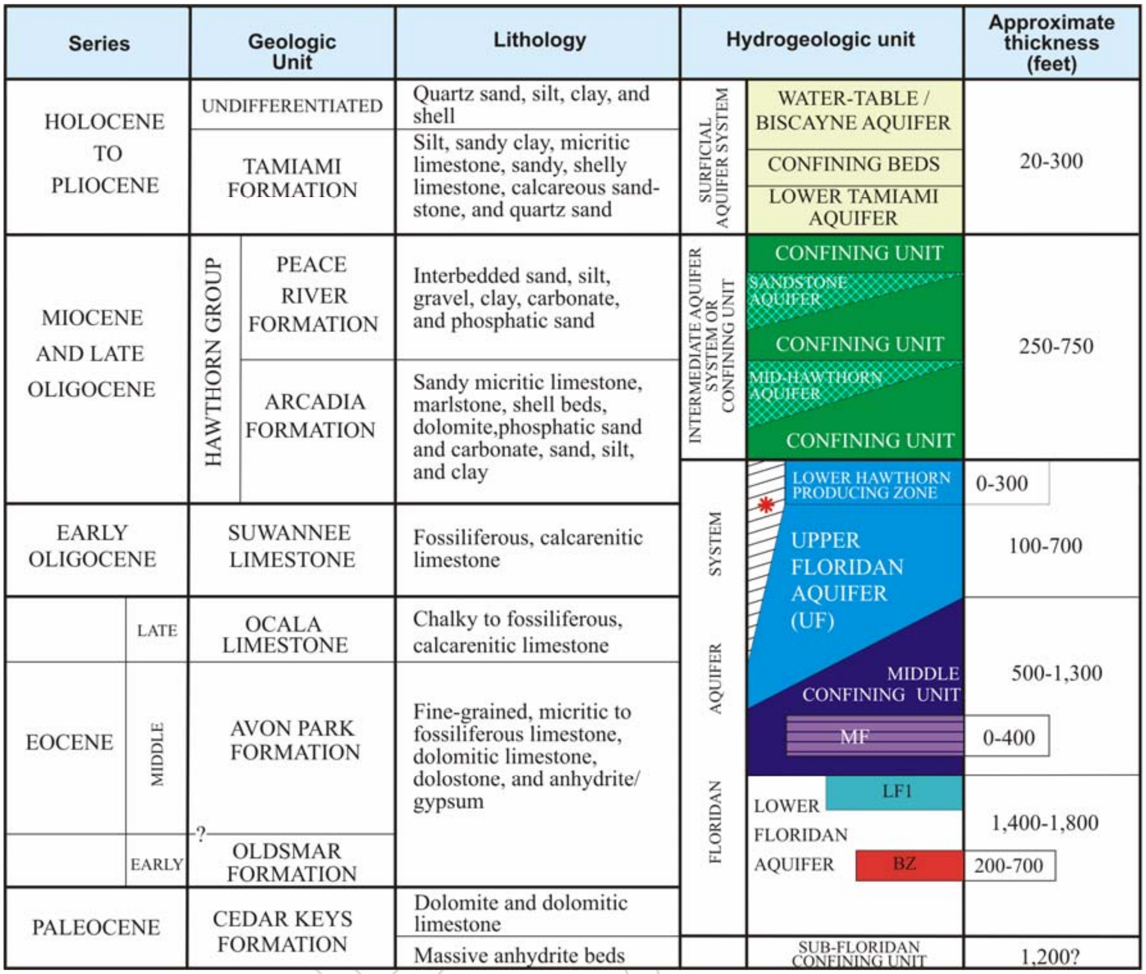

Figure 2-3. Lithology, geologic units and hydrogeologic units (from Reese and Richardson 2004).

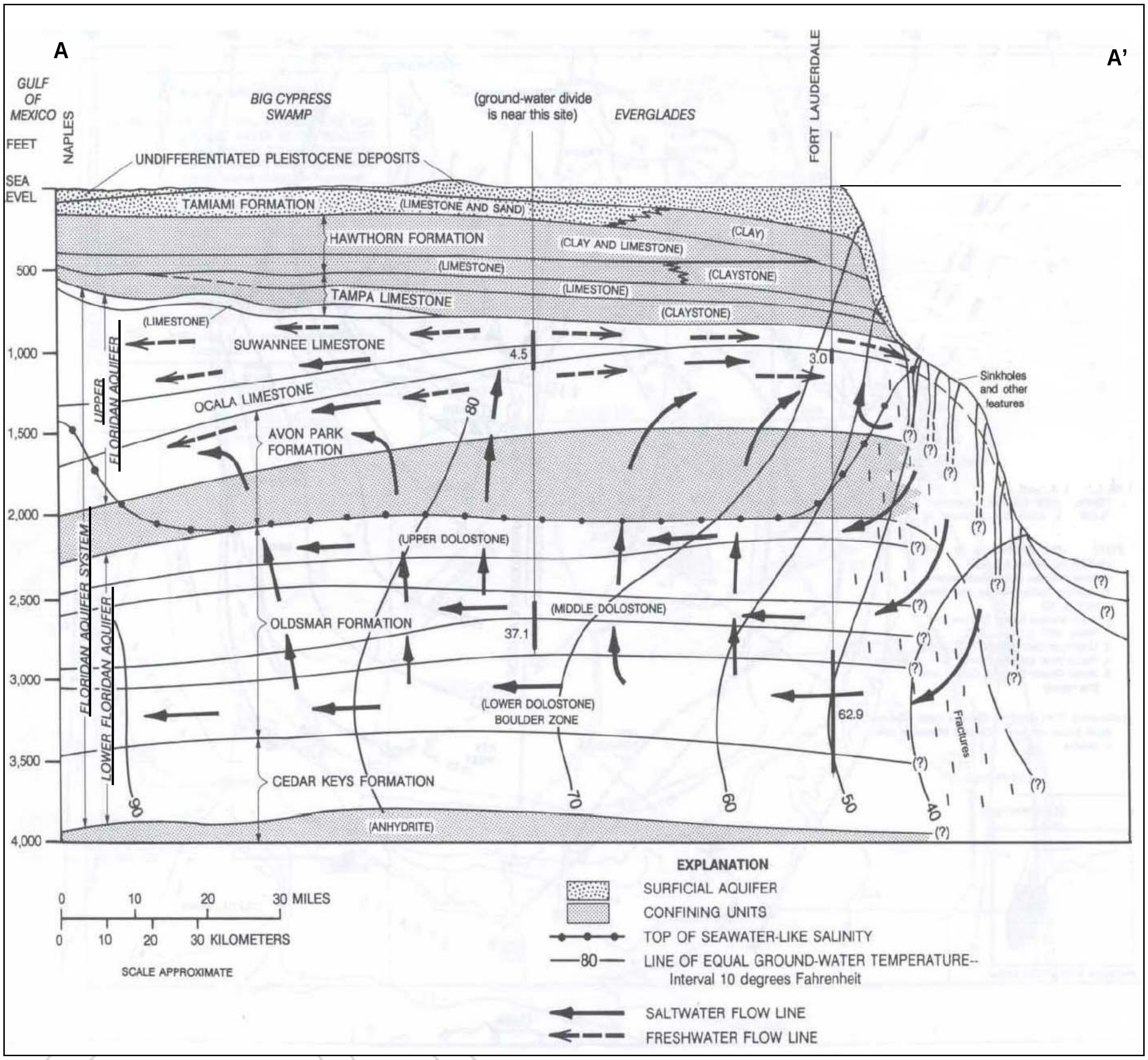

Figure 2-4. Generalized hydrogeologic section A-A' through southern Florida showing isotherms and top of salt water in the sequence of aquifer and confining to semi-confining units (Meyer 1989).

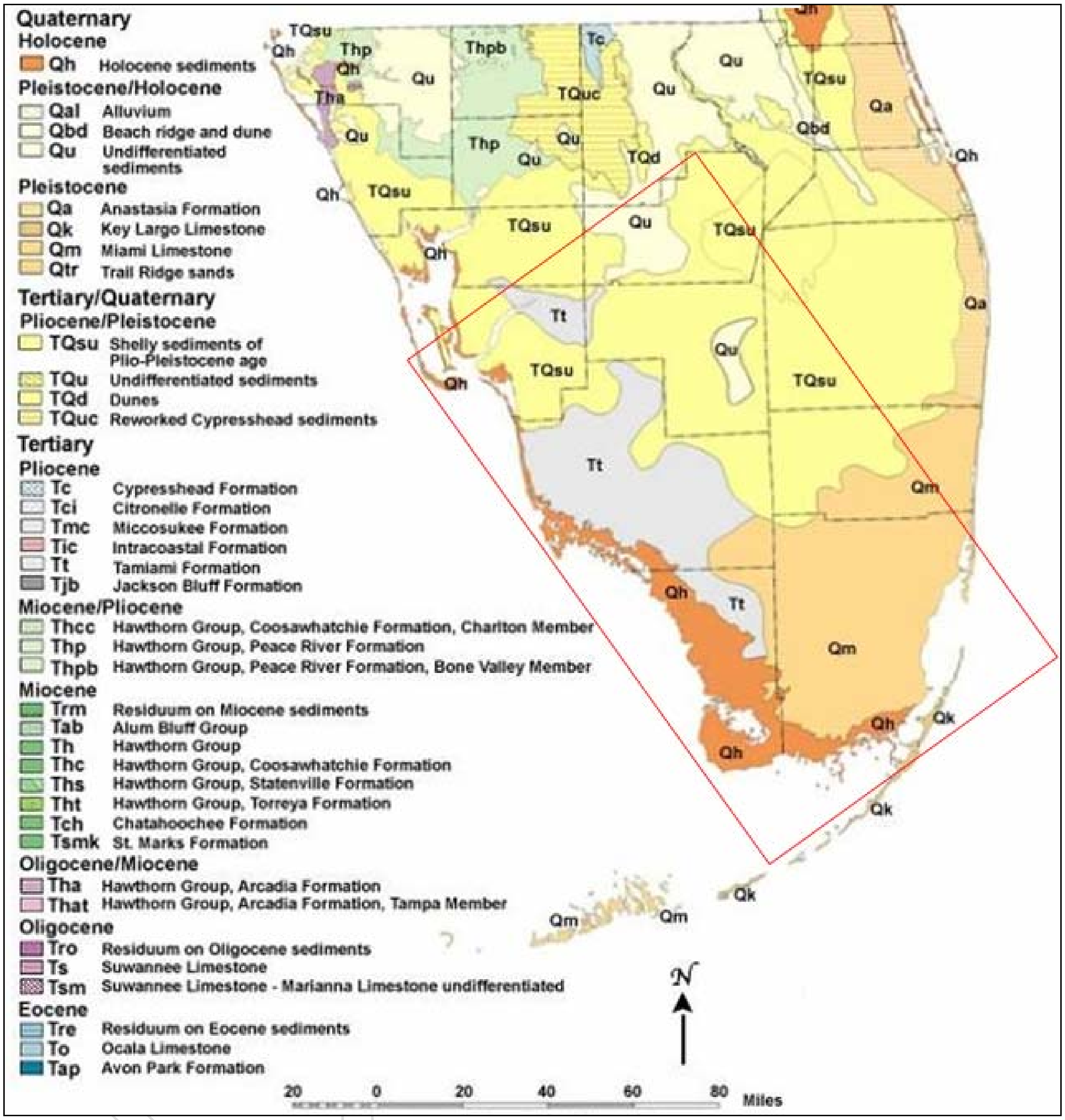

Figure 2-5. Geologic map of the study area (Scott et al. 2001).

Paleocene

Cedar Keys Formation

According to Randazzo and Jones (1997), the Cedar Keys Formation consists of carbonate rocks interbedded with evaporites. Randazzo and Jones (1997) describe the Cedar Keys Formation as being “pervasively dolomitized.”

Miller (1986) further describes the upper third as being cream-colored to grey crystalline dolomite. He reports that the upper portion is highly porous. He describes the lower two-thirds as being composed of finely crystalline to microcrystalline dolomite interbedded with evaporates. The lower portion forms the base of the Floridan aquifer system (FAS). According to Miller (1986), the top of the Cedar Keys Formation ranges from -3,000 to -3,600 feet NGVD within the study area.

Early Eocene

Oldsmar Formation

The Oldsmar Formation is often difficult to identify in south Florida because of diagenetic effects on Early Eocene index fossils such as *Helicostegina gyralis* (Miller 1986). In addition, its lithology is similar to the overlying Avon Park Formation. It is generally located below -2,000 feet NGVD in south Florida. The top of the formation is generally identified by the first occurrence of a dolostone unit below -2,000 feet NGVD. The unit can also be identified with geophysical logs by decreased gamma ray counts and resistivity values and decreased sonic travel times (Bennett 2002). The formation is composed of white to gray limestone interbedded with tan to a light-brown dolostone. Anhydrite and gypsum are also present.

Miller (1986) indicates that the top of the Oldsmar ranges between -1,900 and -2,600 feet NGVD within the study area. According to Miller (1986), the Oldsmar dips to the southwest. The thickness of the Oldsmar Formation ranges from 700 to 1,500 feet and is thickest in Glades, Hendry, and Palm Beach counties (Miller 1986).

Middle Eocene

Avon Park Formation

Within the study area, the Avon Park Formation consists of light brown to black dolomite, fine to medium grained calcarenite, fossiliferous dolomitic limestone with occasional gypsum and anhydrite (Reese and Richardson 2007 in press). The first occurrence of the diagnostic microfossil *Dictyoconus americanus* is also used as a bio-stratigraphic indicator of the Avon Park Formation (Bennett 2004).

The Avon Park Formation is the oldest stratigraphic unit exposed in Florida on the Ocala Platform in Levy and Citrus counties (Scott 2001). The top of the Avon Park Formation ranges from -1,100 to -1,500 feet NGVD. The thickness ranges between 900 to 1,200 feet within the study area (Miller 1986).

Late Eocene

Ocala Limestone

The Ocala Limestone consists of micritic, calcarenitic or coquinoid limestones and occasional dolostones (Reese and Richardson 2007 in press). The Ocala Limestone can be subdivided into lower and upper units based on lithology and depositional environments. The lower unit is characterized by restricted and open-marine carbonate systems. The upper unit is more representative of open-marine, shallow water environments (Randazzo and Jones 1997). Large foraminifera including *Lepidocyclina* *sp. Operculinoides sp. and Camerina sp.* are also present in abundance, mainly in the upper unit (Peacock 1983). In the study area, Reese and Richardson (2007 in press) indicate that the Ocala Limestone becomes dominated by a carbonate mud-rich lithofacies, which reduces the hydraulic conductivity in comparison to the eastern portions of the state.

According to Miller (1986), the top of the Ocala Limestone ranges from -800 feet to -1,200 feet NGVD. It is absent in portions of Broward, Miami-Dade, and Monroe counties. The thickness ranges from 0 to 400 feet in the study area.

Early Oligocene

Suwannee Limestone

The Suwannee Limestone is another generally open-marine carbonate unit dominated by packstones and grainstones similar to the Ocala Limestone. Due to this similarity, it is often difficult to distinguish between the Ocala and Suwannee Limestones although the Suwannee tends to become more clastic towards the top (Randazzo and Jones 1997). Fossils present in the Suwannee Limestone include mollusks, foraminifers, corals and echinoids (Scott 2001).

According to Miller (1986), the top of the Suwannee Limestone ranges between -500 to -900 feet NGVD within the study area. The thickness ranges between 0 to 400 feet. Miller (1986) indicates that the unit is absent in portions of Palm Beach and Broward counties.

Miocene-Pliocene Series

Hawthorn Group

The Hawthorn Group is Miocene in age (Miller 1986) and consists of a diverse mixture of silts, clays, limestones, mudstones, dolomites, quartz sands, and phosphate grains (Reese and Richardson 2007 in press). The Hawthorn Group can be subdivided into the upper siliciclastic Peace River Formation and the lower predominantly carbonate Arcadia Formation, with a potential regional disconformity separating the units (Missimer 1997). Units high in phosphate, easily identified by gamma ray log response (Reese and Richardson 2007 in press), are more prevalent in the Arcadia Formation.

According to Miller (1986), the top of the Hawthorn Group ranges from land surface to -200 feet NGVD. Miller further indicates that the thickness ranges between 300 to 800 feet. The unit is thickest in the southern portion of the study area and thinnest in the northeast portion.

Tamiami Formation

The Tamiami Formation is Pliocene to late Miocene in age (Giddings et al. 2006). Parker and Cooke (1944) state that the unit is primarily composed of sandy limestone, calcareous sandstone, quartz sand, clay, and marl. They further indicate that the Tamiami Formation may contain voids. The lower portion of the Tamiami Formation is more permeable than the upper portion and forms the Lower Tamiami aquifer (Knapp et al. 1986).

Reese and Cunningham (1999) divide the Tamiami Formation into the Pinecrest Sand Member and the Ochopee Limestone Member. They describe the Ochopee Limestone Member as being a fairly permeable unit and form the grey limestone aquifer in south central Florida (Miami-Dade, Broward, Palm Beach, east-central Collier and southern Hendry counties). They indicate that the grey limestone aquifer is the same as the Lower Tamiami aquifer to the north and west. When present, the Ochopee Limestone Member can have a maximum thickness of 130 feet (Reese and Cunningham 1999).

The Pinecrest Sand Member overlies the Ochopee Limestone Member and acts as a confining layer when present (Reese and Cunningham 1999). The Pinecrest Sand member can have a maximum thickness of 130 feet.

Quaternary Deposits

Caloosahatchee Marl

The Caloosahatchee Marl is present in portions of the study area and overlies the Tamiami Formation (Giddings et al. 2006; Randazzo and Jones 1997). The Caloosahatchee Marl is believed to be late Pliocene to early Pleistocene in age. Randazzo and Jones (1997) report that the formation primarily consists of marl, sand, silt, and shells. According to Randazzo and Jones (1997), the Caloosahatchee Marl ranges in thickness between 0 to 25 feet.

Fort Thompson Formation

Randazzo and Jones (1997) report that the Fort Thompson Formation is Pleistocene in age. According to Randazzo and Jones (1997), the unit primarily consists of alternating beds of shells and freshwater limestones, with a maximum thickness of 150 feet. They also report that the unit is fairly permeable.

Other Deposits

Randazzo and Jones (1997) report some other deposits that may have local significance: Pamlico Sand, Lake Flirt Marl, and organic soils. **Table 2-1**(from Randazzo and Jones 1997) describes these deposits.

Table 2-1. Other deposits of significance in southwestern Florida.

Stratigraphic/Hydrologic Unit	Lithology and Water-Yielding Characteristics	Thickness (feet)
Pamlico Sand	Quartz sand; small yields	0-40
Lake Flirt Marl	Shelly calcareous mud; low yields	0–18
Organic Soils	Peat and muck; low yields	0-18

Hydrostratigraphy

The hydrostratigraphy of the study area and model follows that described initially in Reese and Richardson (2004) and finalized in Reese and Richardson (2007 in press), which synthesized regional works into a single viewpoint. The regional works reviewed included: Miller's (1986) comprehensive overview of the FAS (USGS Prof. Paper 1403-B); SFWMD Technical Publication 92-03; Reese's reports in south Florida (WRIR 94-4010, WRIR 98-4253, WRIR 99-4061 and WRIR 03-4242); the FGS 2003 update of the hydrogeology of South West Florida Water Management District (SWFWMD) (FGS, in preparation); and the USGS study of the Lower Floridan aquifer in St. Johns River Water Management District (SJRWMD) by O'Reilly and others (2002, WRIR 02-4193). **Figure 2-**3 depicts the lithology, geologic units, and hydrogeologic units from Reese and Richardson (2004).

Principal Aquifer Systems

Three major aquifer systems underlie southern Florida (**Figure 2-**3) – the SAS, the intermediate aquifer system (IAS), and the FAS.

Surficial Aquifer System

In southwestern Florida the SAS consists of several productive units separated by low-permeability sediments and includes the Water Table aquifer and the Lower Tamiami aquifer. Generally, the Water Table aquifer occurs in the undifferentiated deposits and the upper part of the Tamiami Formation. However, in some areas no undifferentiated deposits are present, and the Water Table aquifer occurs in the Tamiami Formation. The Lower Tamiami aquifer mostly consists of sandy, shelly limestone and calcareous sandstone that occurs in the lower part of the Tamiami Formation (Reese, 2000). The depth of the base of the SAS ranges from 20 to 170 feet below sea level depending on the location (Reese 2000; Bennett 2003).

Intermediate Aquifer System

Aquifers that lie beneath the SAS and above the FAS in southwestern Florida are grouped within the IAS (Southeastern Geological Society Ad Hoc Committee on Florida Hydrostratigraphic Unit Definition 1986).

The IAS lies within the Hawthorn Group and includes, in descending order, the Sandstone aquifer and the Mid-Hawthorn aquifer. The two aquifers tend to be thin in comparison to the thickness of confining units above and below. The Mid-Hawthorn aquifer has been referred to as the Upper Hawthorn aquifer by some previous investigators in southwestern Florida (Reese 2000). The intermediate aquifer system underlying the Lower West Coast region contains multiple productive zones separated by low permeability inter-aquifer confining units (Bennett 2003). The maximum depth of the base of the IAS is approximately 700 feet below sea level (Reese 2000; Bennett 2003).

Floridan Aquifer System

The FAS is defined as a vertically continuous sequence of permeable carbonate rocks that are hydraulically connected in various degrees, and whose permeability is generally several orders of magnitude greater than that of the rocks bounding the system above and below (Miller 1986). The FAS comprises sediments of the Lower Arcadia Formation, Suwannee and Ocala Limestones, Avon Park Formation, Oldsmar Formation, and Cedar Keys Formation. The FAS is divided into four units: the Upper Floridan aquifer, the Middle confining unit, Avon Park permeable zone (Middle Floridan aquifer - MFA), and the Lower Floridan aquifer (LFA) (Bennett 2003).

Upper Floridan Aquifer

The UFA comprises the lower part of the Hawthorn Group, Suwannee, and Ocala Limestones, and the upper part of the Avon Park Formation (**Figure 2-**3). Production zones in the lower part of the Hawthorn Group and the upper part of the Avon Park Formation are not always present. Production zones in the lower part of the Hawthorn Group, if present, are collectively referred to as the Lower Hawthorn producing zone, and they occur in the basal Hawthorn unit from the base of the marker unit to the basal contact of the Hawthorn Group (Reese 2000). In hydrogeologic reports from the SWFWMD, the Lower Hawthorn producing zone is generally identified as production zone three of the IAS (Reese and Richardson 2007 in press). The UFA in the study area generally consists of several thin water-bearing zones of high secondary permeability inter-layered with thick zones of much lower permeability, which is similar to what is found in southeastern Florida (Reese 1994, 2000).

The top of the FAS, as defined by the Southeastern Geological Society Ad Hoc Committee of Florida Hydrostratigraphic Unit Definition (1986), coincides with the top of the vertically persistent permeable early Miocene to Oligocene-aged carbonate sequence. The basal contact of the Hawthorn Group is an unconformity that approximates an important hydrogeologic boundary. Even though the top of the FAS is in places higher than this geologic contact, the most permeable flow zone in the UFA is usually at or near this contact (Reese 2000).

The depth of the base of the UFA is variable, and the base is difficult to define (Reese 2000). Reese and Richardson (2004) place the base of the UFA at 800 feet to

1,500 feet below sea level in most of southwestern Florida; the thickness of the UFA ranges from 100 to 600 feet.

Middle Confining Unit

Below the upper productive unit is a relatively thick, low permeability, semi-confining carbonate unit, formed by the Ocala Limestone and the Avon Park Formation (Bennett 2003).

Avon Park permeable zone (Middle Floridan Aquifer)

The Avon Park permeable zone, also informally known as the Middle Floridan aquifer, lies between the Upper and Lower Floridan aquifers over most of the southern Florida Peninsula. Reese and Richardson (2004) mapped this regional productive zone or sub-aquifer, called the Avon Park permeable zone, which is completely within the Avon Park Formation. This sub-aquifer is well developed in southwestern Florida along and north of the Caloosahatchee River, where it is composed primarily of dolostone, or inter-bedded limestone and dolostone. The majority of its permeability is derived from the fracturing of the brittle dolomite. South of the Caloosahatchee, the unit is comprised almost entirely of limestone as well as the fracturing and associated permeability decrease. The MFA is deemed absent in southern Collier and Monroe counties (Reese and Richardson 2007 in press).

Lower Floridan Aquifer

Miller (1986) described the Lower Floridan aquifer (LFA) as a thick sequence of carbonate rocks containing multiple permeable zones, separated by thick semi-confining units. Reese and Richardson (2004) mapped the top (approximately 1,900 to 2,500 feet below sea level) and thickness (< 10 to >300 feet) of the first permeable zone, and the top of the so-called 'Boulder zone' (2,500 feet to 3,200 feet below sea level) across the entire study area; and (Miller 1986) mapped the altitude of the base of the LFA from 3,700 to 4,100 feet below sea level. The remaining permeable units have been mapped only locally. Most information on this aquifer is derived from deep wells constructed for underground injection of wastewater within the highly transmissive Boulder Zone, which contains massively bedded, cavernous, or fractured dolomitic rocks of high permeability. Because of this, the data is centered in the coastal urban areas. The base of the LFA extends below the Boulder Zone into permeable carbonates of the upper part of the Cedar Keys Formation, below which are massive, impermeable beds of anhydrite (Reese 2000).

HYDROLOGY

Data Collection

Data were mainly obtained from the USGS website, SFWMD, SWFWMD, and National Oceanic and Atmospheric Administration (NOAA). The data from the SFWMD contained information pertaining to water levels, chlorides, pumpage and hydrogeological units. Data were accessed using the SFWMD's Environmental Database (DBHYDRO) and compiled into excel spreadsheets. Data for the FAS, not yet included in the DBHYDRO, were obtained in electronic format from SFWMD staff.

SWFWMD provided water levels, saltwater concentration, pumpage and hydrogeological data solely for Charlotte and Sarasota counties. The data were also obtained in electronic format and contained wells that were located within or nearby the study area of the model.

Tidal data were used to define the boundary condition for the western part of the model domain. Data was therefore collected from the NOAA website. These data contained historical tidal values measured daily for five cities: Everglades City, Indian Key, Flamingo, Naples, and Fort Myers.

The data for hydraulic properties of the Floridan aquifer wells were compiled by the SFWMD (Richardson personal communication). Data were obtained for Collier, Lee, Monroe, Charlotte, and Hendry counties. There was no data available for Glades County. **Figure 2-6** shows the location of wells containing data for hydraulic properties. The range of variation of the initial hydrogeological properties is presented in **Table 2-2**.

Table 2-2. Initial hydraulic conductivity and specific storage in each layer of the LWCFAS Model.

Description	Kx (ft/day)		Kz vertical (ft/day)		Specific Storage (dimensionless)	
	Min	**Max**	**Min**	**Max**	**Min**	**Max**
Water Table aquifer	13.0	18,070.	1.3	1,807.	1.3E-03	1.3E-01
Tamiami confining unit (Upper Tamiami)	0.2	0.2	0.1	0.1	1.0E-07	1.0E-05
Sandstone aquifer (sandstone-clastic/carbonate zone)	2.6	183.	0.3	86.	4.0E-08	7.0E-04
Upper Hawthorn confining zone	0.2	0.2	0	0	1.0E-07	1.0E-05
Mid-Hawthorn aquifer	0.9	1474.	0.1	180.	3.5E-09	1.1E-05
Lower Hawthorn confining zone 1	0.2	0.2	0	0	1.0E-05	1.0E-05
Upper Floridan aquifer (including Lower-Hawthorn aquifer)	4.7	375.	0.9	86.	2.0E-08	8.6E-06
Upper Floridan aquifer (including Lower-Hawthorn aquifer)	0.2	526.	0	1.1	1.0E-08	1.0E-08
Upper Middle Floridan confining unit 1	0.2	0.2	0	5.3	1.0E-05	1.0E-05
Middle Floridan aquifer	0.2	7926.	0	0.2	1.0E-08	3.7E-07
Lower Middle Floridan confining unit	0.2	0.2	0	27.5	1.0E-05	1.0E-05
Lower Floridan aquifer	3.1	4,080.	0.3	408.	2.0E-05	2.0E-05

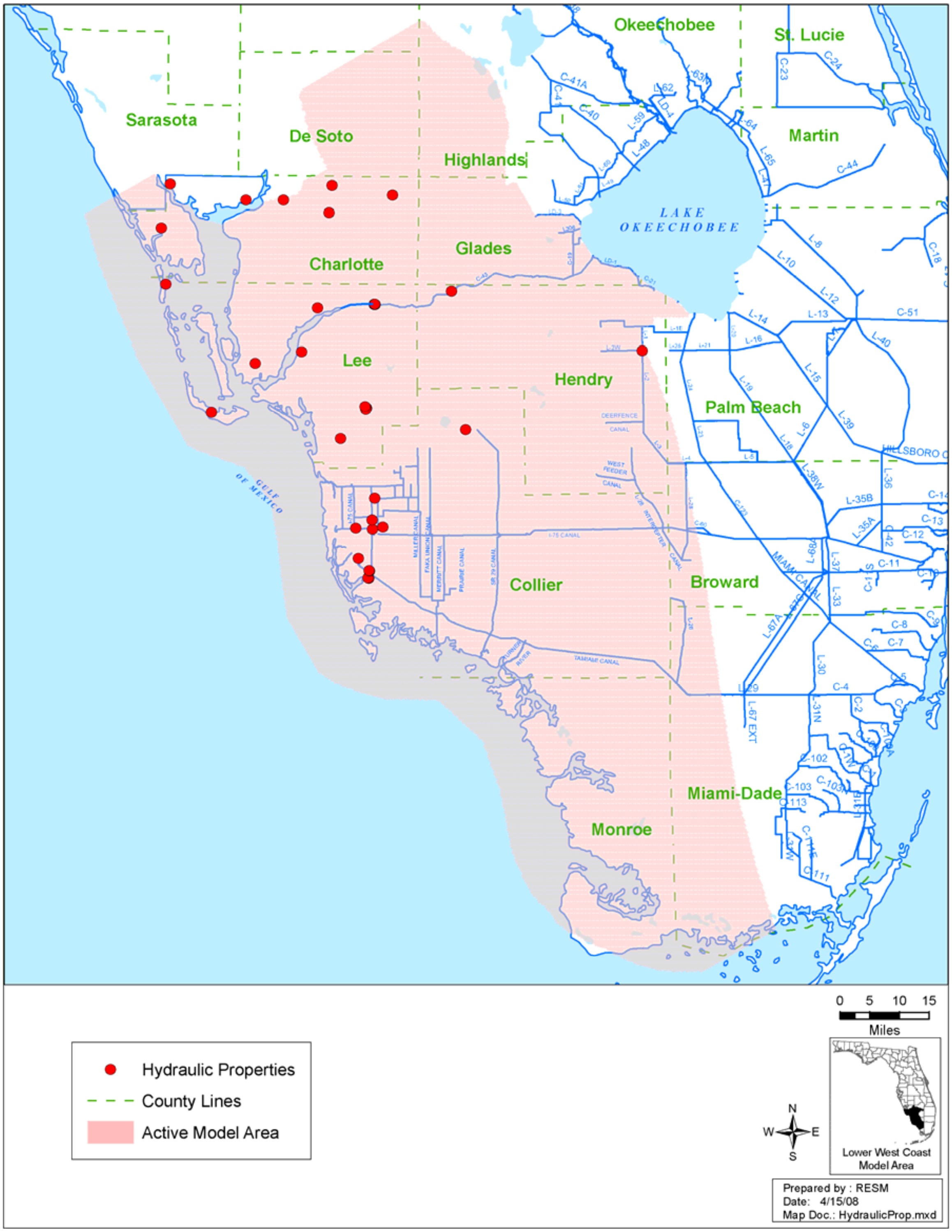

Figure 2-6. Location of wells in the Floridan aquifer system with hydraulic properties.

Hydrologic Stresses

The LWCFAS Model area's major hydrologic stress is primarily due to pumping. With a total of 7,889 pumping wells within the study area, the pumping capacity is approximately 1.1 million cubic feet per day. **Table 2-3** shows pumping distribution within the study area based on aquifer source and use type used in the model. **Figure 2-7** shows the pumping distribution in percentage by aquifer source. The pumping from the Water Table aquifer and surface water is not taken into account in **Table 2-3** and **Figure 2-7**. **Figure 2-8** shows the location of pumpage wells by source aquifer, and **Figure 2-9** and **Figure 2-10** show the pumping location by the water use type. **Figure 2-11** shows the average amount of pumpage from each well for the period 1997-2001.

Water Use

Wells located within the study area are used for both public (PWS) and non-public water supplies (non-PWS). Non-PWS and PWS groundwater withdrawals include domestic, agricultural, livestock, landscape, industrial, irrigation, and aquifer storage and recovery (ASR) uses (**Figure 2-9** and **Figure 2-10**).

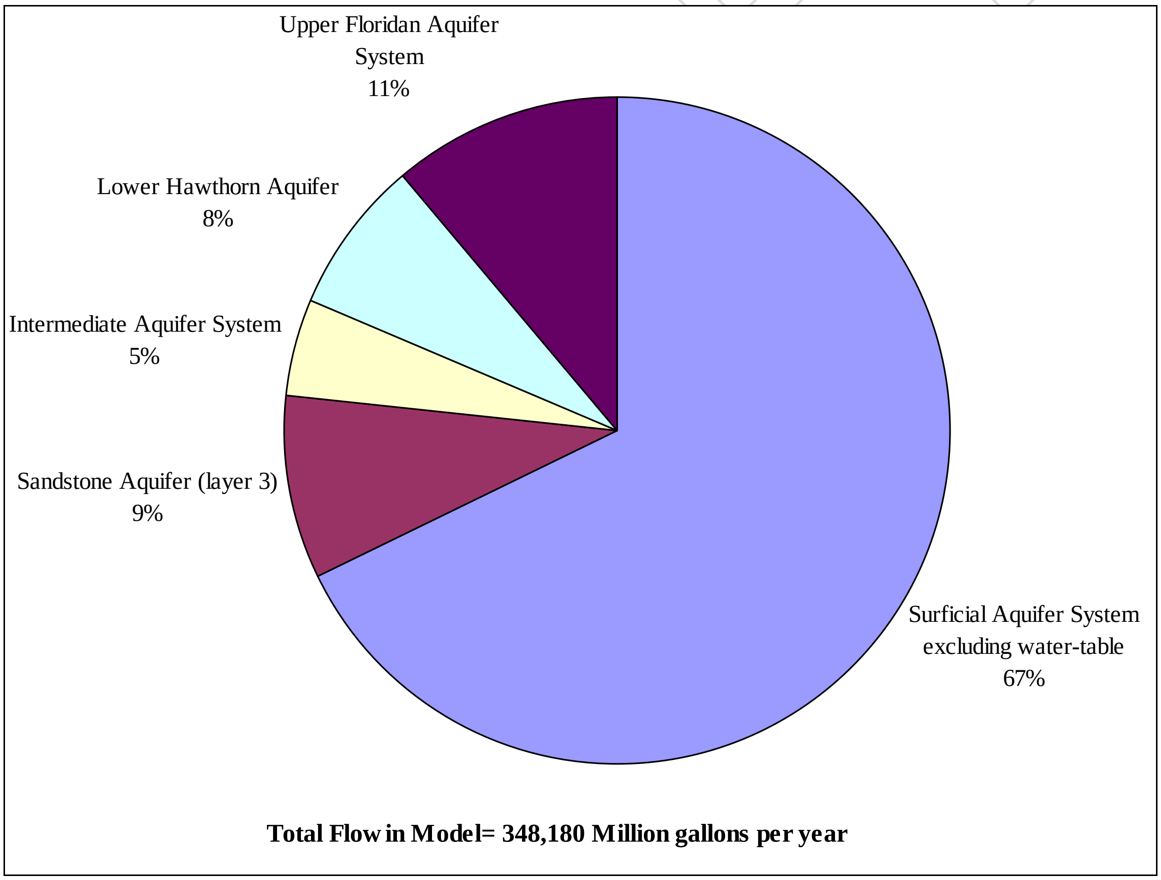

Figure 2-7. Percentage distribution of the total pumping of the LWCFAS Model domain by aquifer source.

Table 2-3. Pumping distribution within the LWCFAS Model study area based on aquifer source and use type.

Aquifer Source and Model Layer	Use Type	Net Pumping (GPD)
surficial aquifer system (Layer 2) excluding water table	AGR	-69,671,420
	IND	-39,908,858
	IRR	-517,589,201
	PWS	-19,812,941
	OTH	-493,775
Total		-647,476,195
Sandstone aquifer (Layer 3)	AGR	-2,923,251
	IND	-3,517,064
	IRR	-77,123,345
	PWS	-1,903
	OTH	-1,097,590
Total		-84,663,153
intermediate aquifer system	AGR	-167,277
	DOM	-12,990,442
	IRR	-19,824,126
	PWS	-5,397,783
	ASR	172,932
	IND	-2,547,807
	OTH	-2,379,260
Total		-43,133,763
Lower Hawthorn aquifer (Layer 7)	AGR	-28,596,818
	IND	-1,105,507
	IRR	-32,501,243
	PWS	-11,480,700
	OTH	-4,527
Total		-73,688,794
Upper Floridan aquifer system (Layer 7 and 8)	AGR	-9,159
	IND	-21,374,721
	IRR	-75,030,556
	PWS	-8,166,417
	OTH	-109,285
	ASR	-264,953
Total		**-104,955,092**

GPD = Gallons per Day
AGR = Agricultural
IND = Industrial
IRR = Irrigation
PWS = Public Water Supply
OTH = Other
ASR = Aquifer Storage and Recovery

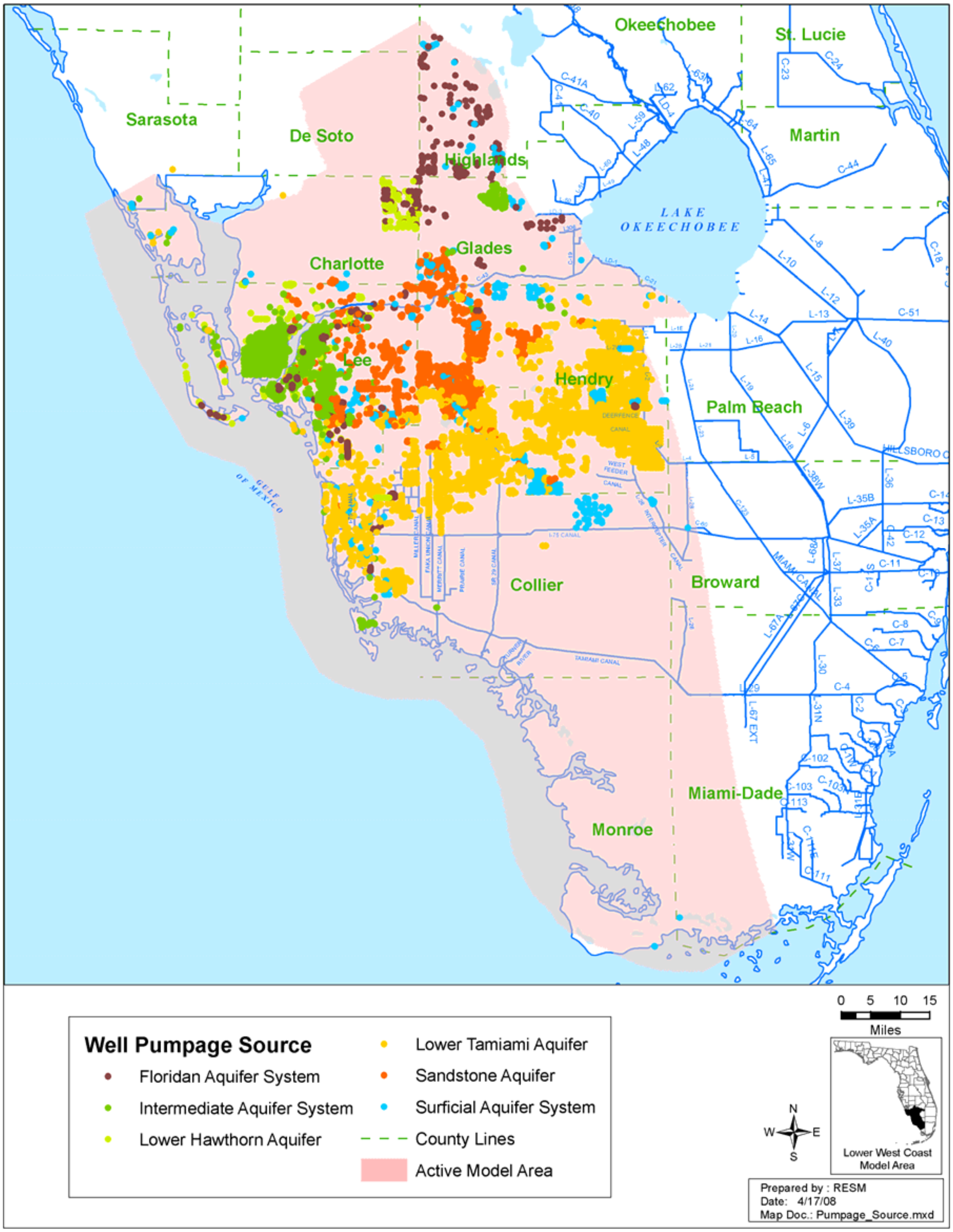

Figure 2-8. Location of pumpage wells by aquifer source.

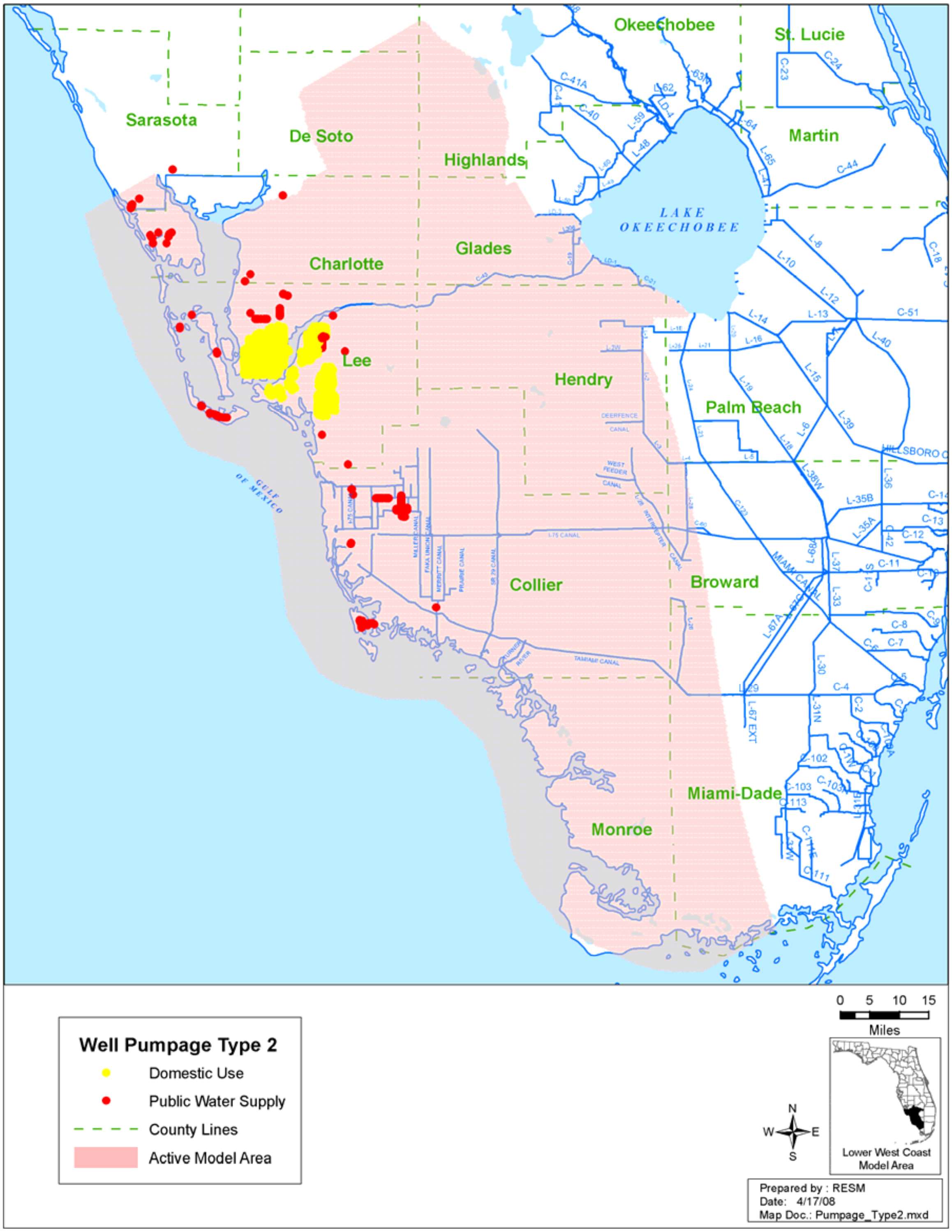

Figure 2-9. Location of pumpage wells for domestic use and public water supply.

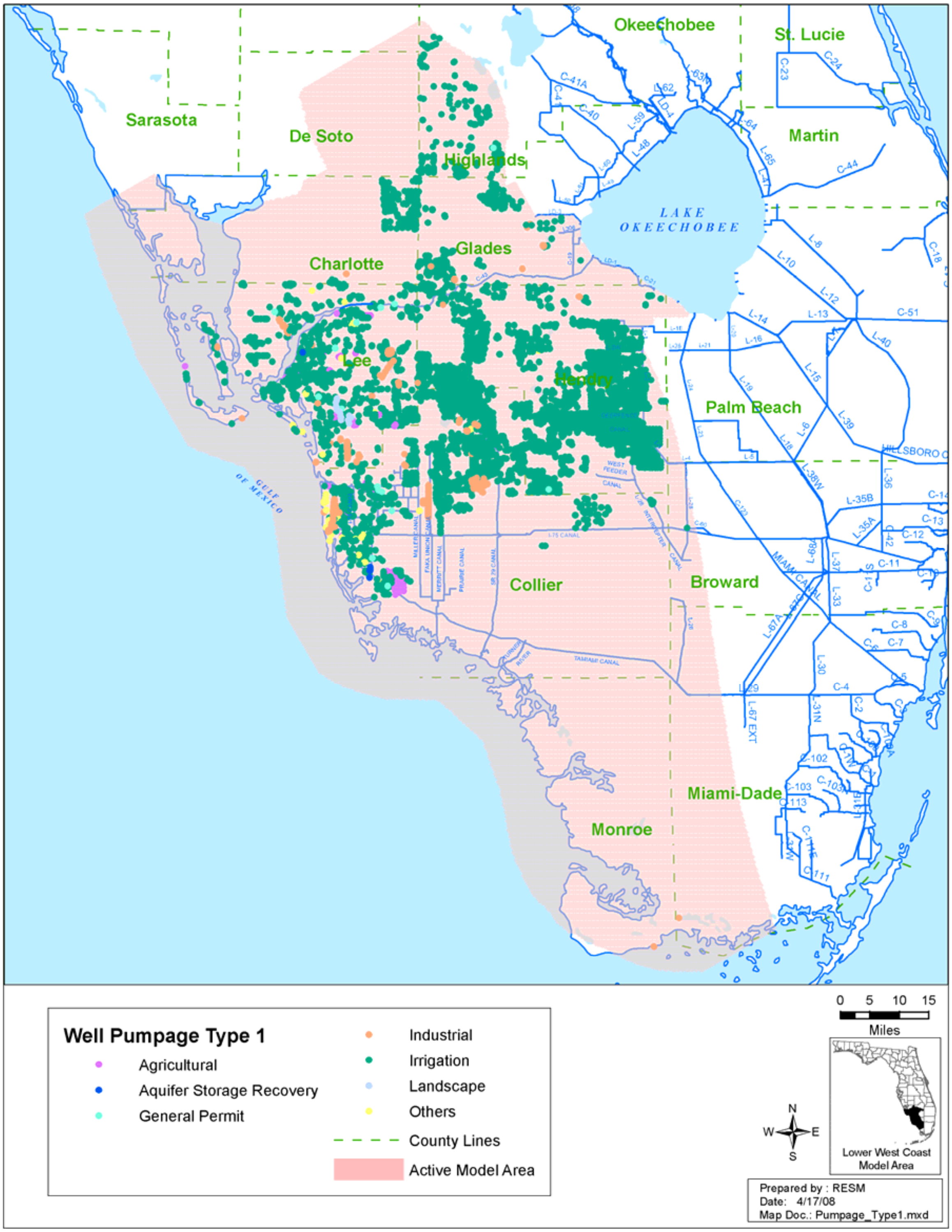

Figure 2-10. Location of pumpage wells by type (excluding PWS and domestic).

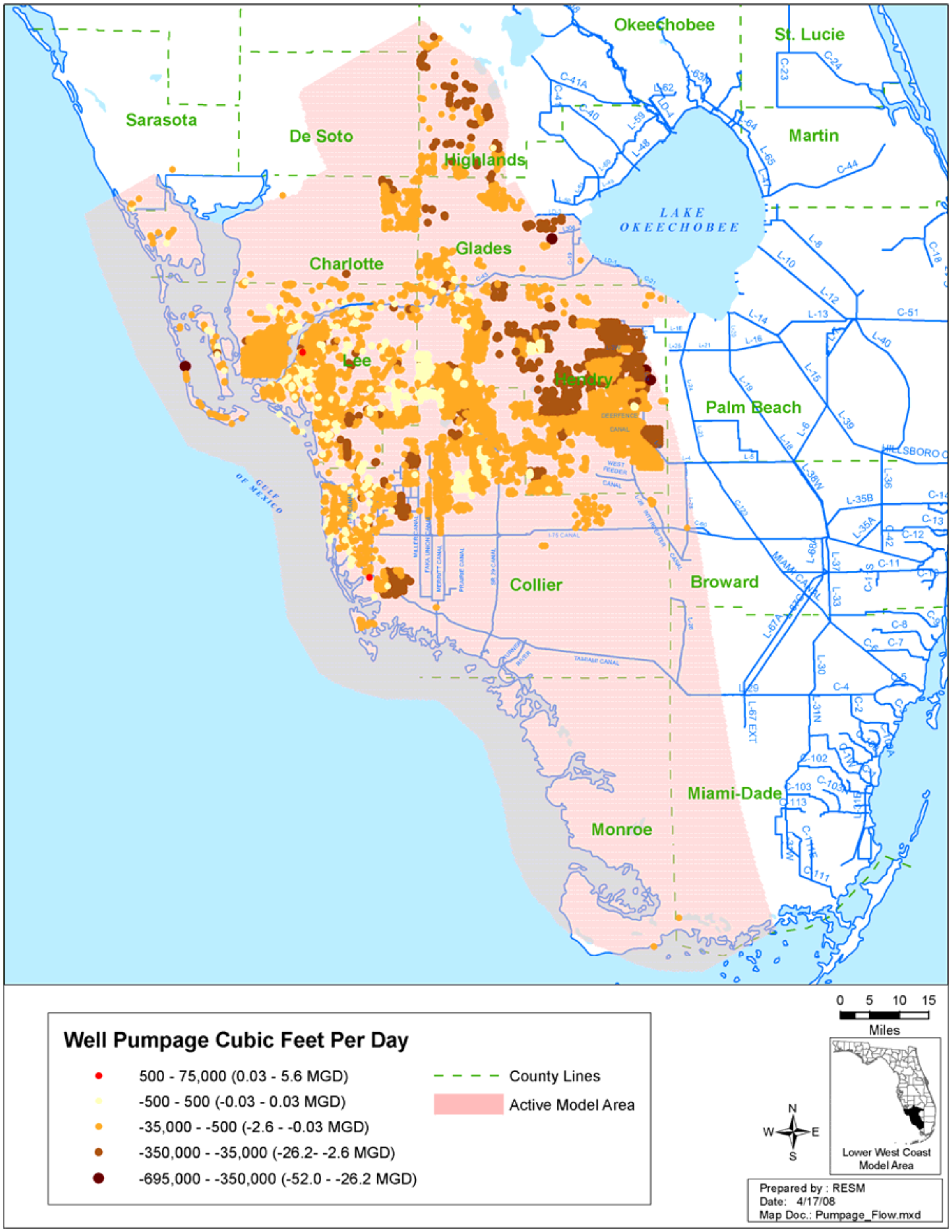

Figure 2-11. Location of pumpage wells categorized by amount of flow.

Water Quality

One of the objectives of the LWCFAS Model is the ability to evaluate the potential for saltwater intrusion. Saltwater intrusion is associated with increased development of coastal aquifers, which forces fresh groundwater that once discharged seaward to be diverted into pumping wells. This causes groundwater levels to decline, which produces a subsequent, landward shift in the seawater/freshwater interface in an attempt to reach a new stable configuration (**Figure 2-12)**. In the case of the LWCFAS, the seawater/freshwater interface may be moving eastward (inland) in some locations. The toe of the interface is estimated to be moving one and a half miles every fifty years, or at a rate of 200 feet to 300 feet per year in Hillsborough, Manatee, and Sarasota counties (SWFWMD 2002).

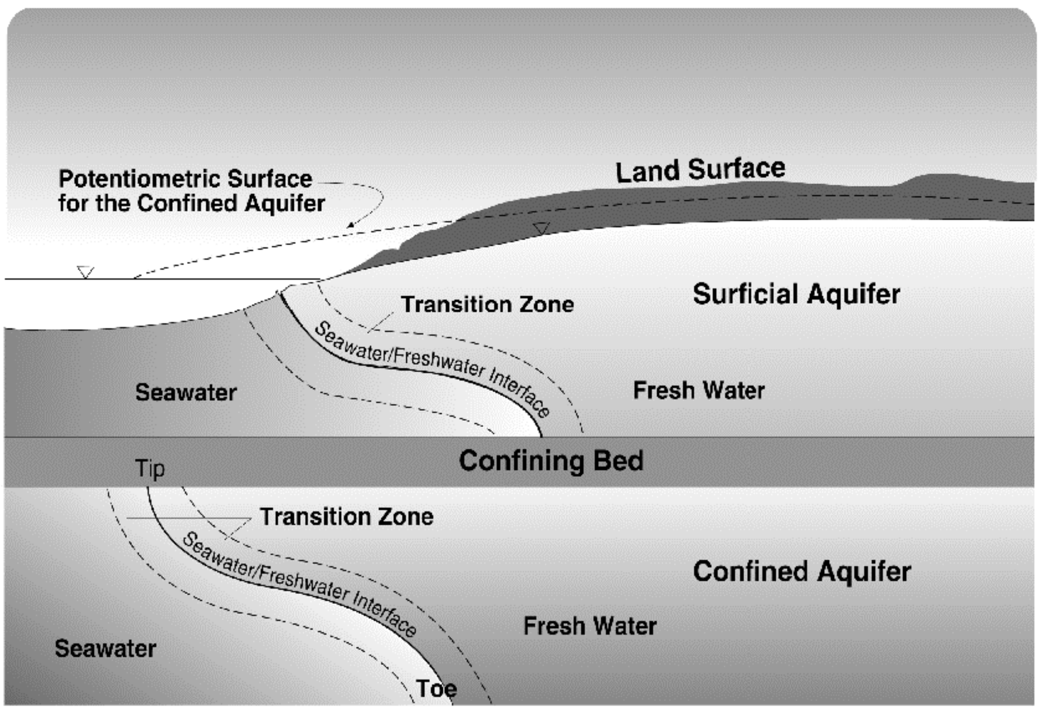

Figure 2-12. Schematic of saltwater-freshwater interface (SWFWMD 2002).

The SAS produces good quality water in most areas of the LWCFAS Model. The LaBelle area and parts of the coast have high concentrations of chlorides and dissolved solids; there are also isolated areas with high iron concentrations. The Lower Tamiami aquifer has been endangered by saltwater intrusion on the coast due to large demands placed on the aquifer (SFWMD 2000).

The IAS has variable water quality, with the Sandstone aquifer being productive in Lee County but only marginally acceptable for potable uses in Hendry and Collier counties. The Mid-Hawthorn aquifer is less productive than the Sandstone aquifer and experiences degradation in water quality as the aquifer dips to the south, west, and east, to yield saline water in much of the LWCFAS Model area (SFWMD 2000).

The FAS yields only non-potable water throughout most of the LWC Planning Region. The quality of water deteriorates southward, increasing in hardness and salinity, of which the latter increases with depth. The Upper Floridan aquifer is the most productive of the FAS and is currently supporting several PWS wells (SFWMD 2000).

Regional Flow System

Groundwater within the study area in the Floridan aquifer system flows laterally through highly permeable zones of dissolution at or near the top of each formation in a southward direction from the area of highest head near Polk City in Central Florida to the Gulf of Mexico and to the Atlantic Ocean as seen in **Figure 2-13** (Meyer 1989).

Surface water and groundwater boundaries in southwest Florida are used to define the study area. The eastern boundary coincides with the groundwater divide of the FAS, while the Gulf of Mexico, 60,000 feet offshore, forms the western boundary of the study area (as depicted in **Figure 2-13**). The northern boundary follows the surrounding area of the Caloosahatchee River, and the southern boundary is defined by the tip of the Florida Bay. Most importantly, the study area encompasses vertically the IAS and FAS. The water table aquifer and Lower Tamiami aquifer are not the focus of this study. The active area of the model is shown in **Figure 2-1**.

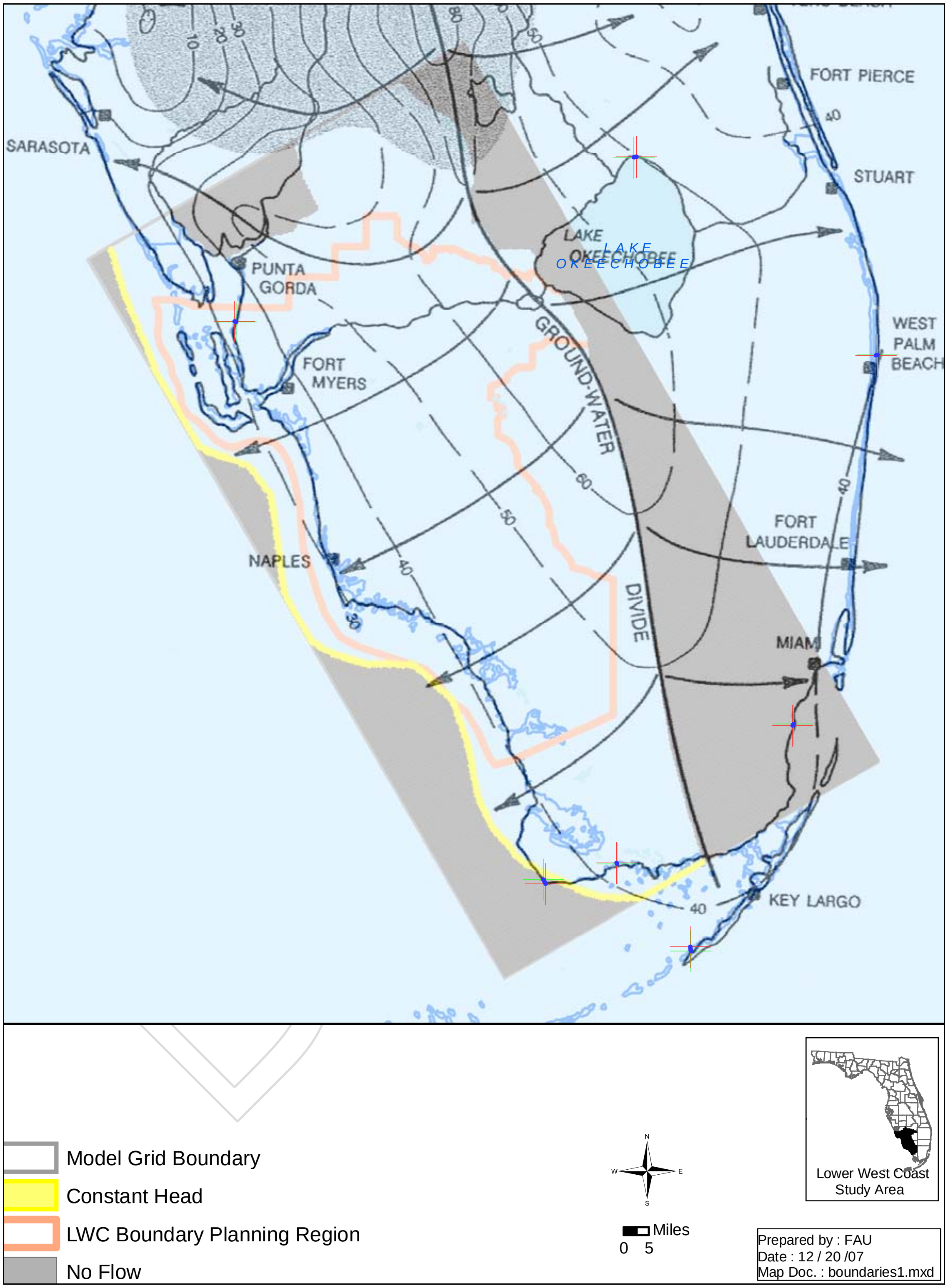

Figure 2-13. Groundwater divide and flow lines of the Floridan aquifer system, LWCFAS Model (modified after Meyer 1989).

CHAPTER 3
SIMULATION OF DENSITY-DEPENDENT FLOW SYSTEM

The Lower West Coast Floridan Aquifer System (LWCFAS) Model, a density-dependent groundwater model, was developed to simulate quasi-steady-state and transient conditions of the Floridan aquifer system (FAS) from years 1997 to 2001. The model will be used to evaluate transient changes to groundwater levels using projected groundwater withdrawals for different model scenarios.

COMPUTER CODE SELECTION

Once modeling objectives have been established and the predominant hydrologic processes within the area of interest have been determined, a model code that can meet the model development and application objectives is selected. A model capable of simulating variable-density groundwater flow and solute transport in three dimensions is needed to study the Floridan aquifer system. SEAWAT-2000, a code created by the U.S. Geological Survey (USGS) (Langevin et al. 2003) was selected for this purpose for the following reasons:

- MODFLOW-2000 (Harbaugh et al. 2000) and MT3DMS (Zheng and Wang, 1999) have been widely accepted in the groundwater modeling profession.
- MODFLOW-2000, MT3DMS and SEAWAT-2000 codes are well-documented and within the public domain.
- SEAWAT-2000 was designed by combining MODFLOW-2000 and MT3DMS into a single computer program.
- Codes are readily adaptable to a variety of groundwater flow systems.
- Codes are modular and facilitate any modifications required to enable their application to the types of unique groundwater flow problems encountered in south Florida.
- MODFLOW-2000, including previous versions, has been widely accepted and customized through the SFWMD's modeling efforts.

SEAWAT-2000 contains all of the processes distributed with MODFLOW-2000 and includes both the Variable-Density Flow (VDF) Process (as an alternative to the density-independent Ground-Water Flow Process) and the Integrated MT3DMS Transport (IMT) Process. These processes may be active or inactive, depending on simulation objectives.

SEAWAT-2000 has two options for dealing with the density terms in the groundwater flow governing equation (Langevin et al. 2003). Both options use a linear state equation representing fluid density as a function of solute concentration. The first option is “uncoupled” and the fastest in terms of computer execution time. In this case, the user may specify either a fluid density array or a concentration array that is held constant during a simulation. The other option calculates fluid densities varying with time. In this option, the flow and transport are “coupled” processes and the fluid density is only a function of solute concentration. For the coupled choice, SEAWAT-2000 contains explicit and implicit options for solving the flow and transport equations. With the explicit approach, the flow equation is formulated using fluid densities from the preceding transport timestep. This approach is adequate for most simulations. For cases with abruptly changing concentrations, the implicit coupling option may provide a more precise solution. With this option, the flow and transport equations are solved repeatedly for each transport timestep until consecutive differences in the calculated fluid densities are less than a specified value. However, the implicit coupling option in SEAWAT-2000 can only be used when an MT3DMS Eulerian approach is selected.

Some of the prominent features of SEAWAT-2000 for the LWCFAS Model include:

- User-specified fluid density arrays. These arrays are used for the variable-density flow equation and are kept constant over time during the entire simulation. This ability aided the calibration process for this model.
- The ability of SEAWAT-2000 to automatically convert input data into equivalent freshwater heads and vice versa before sending it off to output files. This feature eliminates the need for the user to compute equivalent freshwater heads (or vice versa). The output and input both use the observed aquifer head.

The version of SEAWAT, referred to as SEAWAT-2000 in this document, used in the LWCFAS Model is a combined version of MODFLOW-2000 and MT3DMS. It incorporates three of the processes available in MODFLOW-2000: Global (GLO), density-independent Ground-Water Flow (GWF), and Observation (OBS). It also includes two additional processes: Variable-Density Flow (VDF) and Integrated MT3DMS Transport (IMT).

Table 3-1 summarizes the different processes used for the LWCFAS Model. The VDF Process was designed to solve the variable-density groundwater flow equation using the approach outlined by Guo and Langevin (2002). The IMT Process solves the solute-transport equation by integrating the MT3DMS packages directly into the MODFLOW-2000 program. A revised version of GLO interacts with the MT3DMS mechanism between flow and transport, and a similarly modified OBS works with the VDF Process; however, the OBS still needs further programming to work smoothly with solute concentrations (Langevin et al. 2003). In any event, the OBS is not used in the LWCFAS Model. The main reason for integration with the MT3DMS mechanism is to allow variable-density simulations where the flow and transport processes are coupled, and hence, the flow and transport equations need to be solved simultaneously (i.e., implicitly) for each timestep or sequentially (i.e., explicitly) using one timestep lag (timestep here specifically means MODFLOW timestep).

Overall, the SEAWAT-2000 program structure, input, output, and execution conform to MODFLOW-2000 conventions. Specifically, packages and processes are activated for a SEAWAT-2000 simulation using a “name file”. This provides users with the capability to change simulation options without having to change the input files or computer programs.

The Global (GLO) Process controls overall program execution by reading options from the name file, opening files, and reading information about space and time discretization. The original MODFLOW-2000 GLO Process was modified to add SEAWAT-2000 functionality. Changes were made to implement the transport timestep.

Table 3-1. Processes available in SEAWAT-2000.

Abbreviation	Description
GLO1	Global Process
GWF1	Ground-Water Flow Process
VDF1	Variable-Density Flow Process
OBS1	Observation Process
IMT1	Integrated MT3DMS Process

SEAWAT-2000’s ability to use the VDF Process without simulating solute transport could be applicable to coastal groundwater flow models that require accurate representation of the ocean boundary, but do not require simulation of saltwater intrusion. This approach can substantially shorten computer run times because timestep lengths are not restricted by stability criteria that are necessary for accurate transport solutions.

Like most finite-difference modeling codes, SEAWAT-2000 may have some shortcomings for simulating flow and/or transport in karstic environments. SEAWAT-2000 assumes that Darcy’s Law is valid and that Fick’s Law is appropriate for simulating dispersive transport. Fractures and solution cavities may be represented using high hydraulic conductivities to simulate the decreased resistance to groundwater flow that these features represent. However, simulated groundwater flow velocities may be less than actual velocities in fracture/karst zones, and the simulated transport of dissolved solute in fracture/karst zones may be less than the actual movement. Indeed, in fracture/karst zones, there is a limitation in the ability of SEAWAT-2000 to accurately simulate the upward movement of saline water from the LFA to the UFA (and from the UFA upward) through these zones, as no one fully knows where said fractures truly exist. Some areas of increasing chloride concentrations and relatively high temperatures in the UFA correspond to a fault trace mapped by Barnett (1975) and Walker (2008), which suggests that vertical groundwater flow may be seeping upward through fractures.

Special Discretization

SEAWAT-2000 simulates groundwater flow in aquifer systems using the finite-difference method. The aquifer system is divided into rectangular or quasi-rectangular blocks by a grid (**Figure 3-1**). The grid of blocks is organized by rows, columns and layers, and each block is commonly called a cell.

For each cell within the aquifer system, the user must specify aquifer properties. In addition, the user specifies information relating to wells and other hydrologic features for the cells corresponding to the locations of the features. For example, if the interaction between a boundary and an aquifer system is simulated, then for each cell traversed by the boundary, the required input information includes layer, row, and column indices, boundary stage, concentration, and hydraulic properties of the cell. In addition, SEAWAT-2000 allows the user to specify which cells within the grid are part of the groundwater flow/transport system and which cells are inactive (e.g., outside of the groundwater flow system).

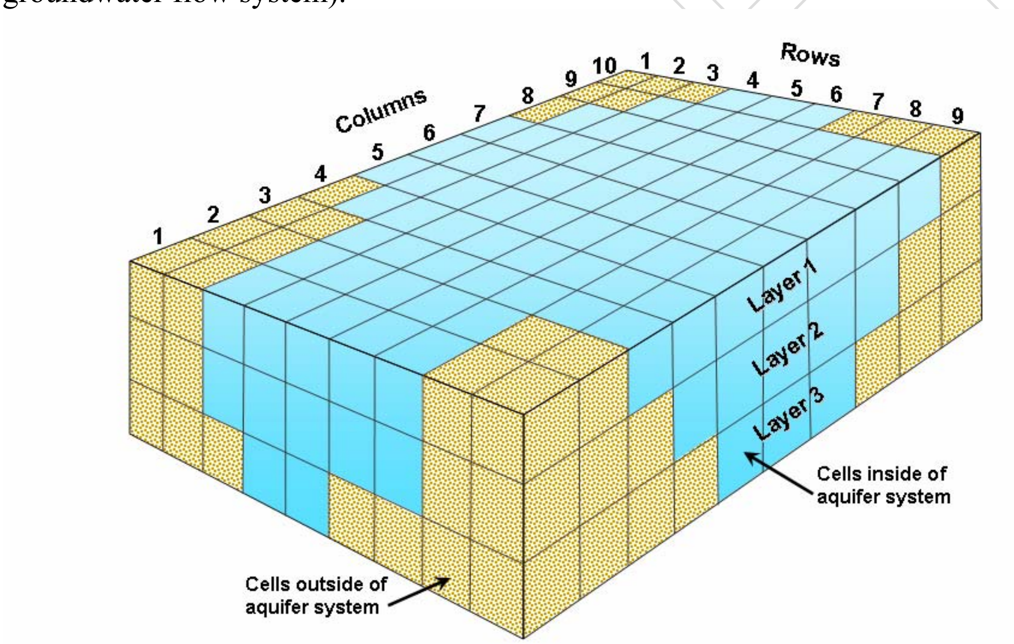

Figure 3-1. Example of model grid for simulating three-dimensional groundwater flow.

Temporal Discretization

SEAWAT-2000 time discretization depends upon active simulation modes. Simulation modes without solute transport use the standard MODFLOW method. However, in simulation modes that contain solute transport, each simulation is divided into stress periods that, in turn, can be subdivided into flow timesteps. In simulation modes that contain solute transport, flow timesteps are further divided into transport timesteps for the simulation mode that contains solute transport. In order to successfully save results from the simulation, the final transport step generated must correspond with the end of a flow timestep. The same convention applies for variable-density simulations with SEAWAT-2000. When running an implicit coupled model, the lengths of transport timesteps, which are the same as flow timesteps in an explicit coupled model, are calculated based on stability criteria.

SEAWAT-2000 INCLUDING SFWMD SOURCE CODE

SEAWAT Packages Applied in the LWCFAS Model

The SEAWAT-2000 source code consists of a main program and a series of independent subroutines called modules. The modules, in turn, can be grouped into packages. Each package, in general, deals with a particular hydrologic/transport process or solution algorithm. The packages used for LWCFAS Model simulations, including those developed or enhanced by the SFWMD and/or FAU, are shown in **Table 3-2**. The original packages that form SEAWAT-2000 are well-documented in their accompanying user manuals, Langevin et al. (2003), MODFLOW 2000 (Harbaugh et al. 2000) and MT3DMS (Zheng and Wang 1999). Therefore, the original packages are not actively discussed herein.

Additional SEAWAT Packages Applied

The modular structure of SEAWAT readily allows for modifications or the creation of additional packages. The SFWMD and FAU have taken advantage of this feature and developed several additional packages, which are described in this section. Additional information about these packages is readily available at the SFWMD website. (i.e., http://www.sfwmd.gov/)

The Utility Generation Package (UGEN)

The Utility Generation package (UGEN) was developed by the Geosciences Center at FAU to generate time-related MODFLOW input during model execution. Traditional MODFLOW input files must be developed prior to execution for each package and for the entire simulation period. UGEN creates input files "on the fly" by linking the static input parameters, such as physical location, with the dynamic temporal data, much like a relational database (Restrepo et al. 2003). The "location name" identifiers link the static and dynamic data. UGEN can be used to generate the following MODFLOW-2000 packages: River (RIV), Drain (DRN), Well (WEL), General Head Boundary (GHB), Reinjection Drain Flow (RDF), Time-Variant Specified-Head (CHD), and Diversion (DIV). It can also be used to correct heads due to the presence of the saltwater interface and to calculate the hydraulic conductance for the River, General Head Boundary, and Drain packages.

Generating the input with UGEN increases the functionality of MODFLOW by reducing execution time and storage requirements. UGEN is compatible with the modular structure and programming language (FORTRAN) of MODFLOW. When activated within MODFLOW, UGEN saves both storage space and execution time. The placement of the static data and time-series data into separate files also reduces model setup time and facilitates quality assurance and quality control (QA/QC) of input information.

Table 3-2. SEAWAT packages used in the LWCFAS Model.

Process	Package or Filename	Description	Notes
GLO	Global (GLO)	Controls program, opens files, and reads global data (space/time discretization)	Developed by USGS
	Discretization (DIS)	Handles time and space discretization	
GWF-VDF	Variable-Density Flow (VDF)	Converts aquifer head to equivalent freshwater head (i.e., fresh water to salt water and vice versa)	Main SEAWAT package (USGS)
	Basic (BAS)	Specifies initial heads and active zones	
	Layer-Property Flow (LPF)	Specifies anisotropy, layer types, and hydrogeologic data for each layer	Properties derived from geologic data (USGS)
	General-Head Boundary (GHB)	Simulates groundwater flow/solute exchange between selected cells and specifies boundary as a function of water level difference and boundary properties	Based on measured stages or interpolated stages that are assigned in conjunction with UGEN and HBXY
	Constant Head (CHD)	Simulates groundwater flow/solute exchange between selected cells and prescribed heads/concentrations	
	Well (WEL)	Simulates public water supply (PWS), agriculture (AGR), aquifer storage and recovery (ASR) and other groundwater withdrawals	Based on measured flows that are assigned with UGEN
	Utility Generation (UGEN)	Creates input files during model execution by linking static data with time series data	Generates input for WEL, GHB and CHD; developed by FAU
	Observation (OBSG)	Generates plots for calibration	Developed by FAU
	Boundary Head Interpolation (HBXY)	Interpolates heads for GHB, CHD and initial conditions	Generates input for GHB and CHD; developed by FAU
	Pre-conjugate Gradient (PCG)	Solution option	Developed by USGS
IMT	Basic Transport (BTN)	Basic tasks required by entire transport model. Among these tasks are: problem definition, boundary specification, initial conditions, of the step size determination, mass balance and printout information	Initial concentrations and active zones; developed by Zheng and Wang
	Advection (ADV)	Solves concentration change due to advection with an explicit scheme or formulates advection coefficient matrix term for matrix solver	Developed by Zheng and Wang
	Dispersion (DSP)	Allows inclusion of three-dimensional multi-component dispersion coefficients in transport simulation. User specifies one dispersion coefficient for each mobile solute component at each model cell	Dispersivity developed by Zheng and Wang
	Source-Sink Mixing (SSM)	Represents solute mass entering/leaving model domain through sources/sinks. Point sinks/sources include wells, constant-head and general head dependent boundaries	Flow rate and concentration developed by Zheng and Wang
	Generalized Conjugate Gradient	Solution option	Developed by Zheng and Wang

When MODFLOW is executed with UGEN, three input files are needed. The first, the UGEN file, defines the number of stations for stages and/or flows and any flags activate UGEN for any MODFLOW package with dynamic input data. The second type of input file needed is the observation file. UGEN observation files contain stage and/or flow values for each stress period for all stations. Stress periods are essentially the rows, with the stations listed across each row like columns, as shown in **Table 3-3**.

Table 3-3. Example of UGEN observation file displaying time-varying data (e.g., stages).

ID	Year	Month	Day	Station-1	Station-2	Station-3
1	1990	1	1	14.3	7.9	11.1
2	1990	1	2	14.5	8.1	11.5
3	1990	1	3	14.5	8.0	10.8
4	1990	1	4	14.3	8.3	11.0

The third type of input file is the modified MODFLOW input package file to be used with UGEN (e.g., RIV, DRN, WEL, GHB, DIV, RDF, CHD, or HBXY). This input file will provide the same information that MODFLOW requires. However, instead of having stage(s) or flow(s) values, it will have the location name identifier (The location (station) name must be provided with a length of no more than 21 characters). This represents the "static" portion of the UGEN input files that the utility links with the "dynamic" information provided in the observation files. These modified MODFLOW input files may be kept constant during all simulations, or may be changed if necessary. The UGEN package has already been implemented in SEAWAT-2000. The UGEN package also includes an option to "jump" records in the UGEN time series. For example, if the input time series has daily records and one wants to run a weekly simulation, there is no need to change the original time series. A flag in the UGEN tells the program to skip a given amount of records so the program will run stress periods on a weekly basis, or the desired stress period. In this case, flows are averaged within UGEN during each stress period. Nevertheless, the user has to be aware of matching the new number of stress periods and stress periods lengths in the DIS and BTN files. This option is quite useful for calibration/simulation purposes where the model may be run with different stress period lengths.

The Interpolation Head Boundary Package (HBXY) for the Groundwater Flow Model, MODFLOW-2000

The Interpolation Head Boundary package (HBXY) was developed by the Geosciences Center at FAU to interpolate MODFLOW input spatially for each stress period during model execution. HBXY interpolates the heads in the input files "on the fly" by linking the static input parameters, the physical location (X,Y coordinates), with the dynamic temporal data, much like a relational database. The "location name" identifiers link the static and dynamic data. HBXY can be used to generate the model initial conditions and to generate these MODFLOW-2000 packages: GHB and CHB.

HBXY must be used with UGEN. The HBXY also has the ability to vary stress period length using the UGEN daily time series.

Generating the input with HBXY increases the functionality of MODFLOW by reducing the pre-processing. HBXY is compatible with the modular structure and programming language (FORTRAN) of SEAWAT-2000.

Simulation Modes (Coupled/Uncoupled)

In SEAWAT-2000, there are two main simulations modes: coupled and uncoupled.

For the former, the model can simulate coupled variable-density flow and solute transport; in this mode, fluid density (as used in the VDF Process) is calculated by using a state equation in concert with the simulated solute concentration. For many problems involving coupled flow and transport, users should be aware that computer run times might be exceedingly long because timestep lengths are subject to the many stability criteria necessary for finding accurate transport solutions.

In the uncoupled mode, flow and transport are (as the name implies) uncoupled, meaning that the flow solution is affected only by the user-specified density array (which is constant in time but not in space). Thus, the flow field is not affected by the solute concentrations simulated with the IMT Process, which translates into a huge decrease in computation times. This option allows a representation of the density-dependent boundary as a steady distribution of concentrations in space, thus allowing the user to simulate a stationary saltwater interface or a density-dependent flow, as per the particular user's needs.

Two LWCFAS models were developed: one coupled and another uncoupled. During a 5-year simulation, the density field did not change appreciably in the coupled model; nevertheless, if the model is left running for an extended period of time (not less than 10,000 days) such that a dynamic equilibrium is reached, the resulting density distribution may indeed change. Consequently, the user should be cognizant of the fact that the resulting potentiometric head would also vary.

Under the horizontal and vertical discretization previously described, a typical simulation (using the 12,000 feet by 12,000 feet cell uncoupled model) requires an average of approximately 0.6 seconds of CPU time per timestep. The 3,000 feet by 3,000 feet cell uncoupled model requires approximately 18 seconds of CPU time per timestep. Both cases use a 3.2 GHz Intel Xeon processor with 4 MB RAM. The simulation was also run for both of the aforementioned models using a coupled (as opposed to uncoupled) scenario; in this case, approximately 18.5 seconds of CPU time per timestep was needed for the former and 517 seconds for the latter.

LWCFAS MODEL DESIGN

Model Grid

A finite-difference model grid was designed so that the model columns would roughly parallel the southwest coast and the model rows would be aligned with the principal direction of groundwater flow. The degree of rotation was selected by using the regional flowlines defined in the Floridan aquifer system, depicted in **Figure 2-13**. When groundwater flow is parallel to one of the primary model axes, problems with numerical dispersion that result from solving the transport equation are reduced.

The model domain is a rectangle with direction, northwest to southeast. The rotation angle from the north was counterclockwise by 30 degrees. The grid was bounded on the northwest by Highlands, Hardee, De Soto and Sarasota counties; on the northeast by Highlands, Glades, Hendry, Palm Beach, Broward and Miami-Dade counties; on the southeast by the bottom of the Florida Peninsula; and on the southwest by the Gulf of Mexico. The grid limits (shown in **Figure 2-1 and Table 3-4**) in the U.S. State Plane Florida East HARN 83 feet are:

Table 3-4. Model grid limits.

Corner	X Cell Center	Y Cell Center	X Cell Corner	Y Cell Corner
North	541613.36	1159147.87	542743.91	1162892.28
South	586098.08	194098.08	585188.58	190201.95
East	970613.36	416098.08	974472.78	414909.02
West	157098.08	937147.87	153459.72	937769.09

Two versions of the grid are available for the LWCFAS Model. The first model domain is discretized into 72 rows and 37 columns, with a uniform cell-size of 12,000 feet by 12,000 feet. The second model grid is discretized into 287 rows and 150 columns, with a uniform cell-size of 3,000 feet by 3,000 feet. The former was used for semi-automatic calibration purposes while the latter served as the main simulation model grid. The summary of the LWCFAS Model input data is presented in **Appendix A**.

Spatial and Temporal Discretizations

Horizontal Discretization

In order to represent all the features of the hydrogeologic system with acceptable accuracy, the production (or simulation) model's spatial discretization was set to a uniform grid 3,000 feet long by 3,000 feet wide (9,000,000 square foot cells) for a total area of about 13,882 square miles. However, for modeling purposes, 14,326 cells were set as inactive and 28,724 as active for an approximate active area of about 9,254 square miles. The spatial discretization was set to a uniform grid of 12,000 feet long by 12,000 feet wide when the model was undergoing calibration. In both versions, the active zone is defined, when possible, as larger than the Lower West Coast (LWC) Planning Area, such that a buffer zone is created around the study area.

Vertical Discretization

Simulation of a density-dependent system requires a relatively fine level of discretization in the vertical direction. The model grid consists of 12 layers defining the aquifer systems. The top and bottom layers of the model were represented by constant head boundaries and hence the recharge and evapotranspiration processes were not required.

The constant head boundary in Layer 1 represents the interaction of the water table aquifer with any surface water bodies and contains enough measured data in space and time to obtain reasonable estimates of the heads and concentrations. Layer 12 represents the Lower Floridan aquifer (LFA). Measured data in the LFA are lacking; therefore, a few known points and educated suppositions were used to define this boundary, as described in the next section. Since the main goal of the project was to focus on the UFA (and to some extent on the intermediate aquifer system), it is reasonable to assume that the interpolation technique used to generate the constant head boundary for Layers 1 and 12 had a relatively minor effect on target layers. This is mainly because the UFA layers are isolated from the top and bottom layers by layers of low hydraulic conductivity (thick confining units). Lake Okeechobee may also have an effect on the behavior of the aquifer systems, including the FAS; however, only Layers 1 through 3 extend eastward to the lakeshore.

The data (Richardson 2005; Reese and Richardson 2004) for the top and bottom surfaces were provided by the SFWMD and the USGS in the form of an evenly-spaced grid. The surfaces were updated with new data for the FAS provided by the SFWMD (Richardson 2006). **Table 3-5** shows that the SFWMD mapped the UFA by the surfaces, Upper Floridan top (UFtop) and Middle confining unit top (MCtop); however, for modeling purposes, the UFA was split evenly into two model layers (7 and 8) in order to have a better vertical resolution for the transport model. The primary change performed to the data sets was to assign a minimum thickness of 15 feet. In portions of the modeling zone where the aquifer does not exist or is pinching out, layers were altered, including the bottom of the Lower Floridan (LFbot) and the bottom of the Middle Floridan (MFbot) (Avon Park permeable zone). Therefore, the final surfaces were practically equal (approximately less than 10 feet different) to the original elevations. The vertical discretization of the multi-aquifer system is shown in **Table 3-5.** The top/bottom surfaces are included in the metadata and are used as model input.

A neighborhood of 15 cells was used for the averaging of the top and bottom surfaces of Layers 1, 3, and 5 (corresponding to the water table aquifer, Lower Tamiami aquifer, Sandstone aquifer and Mid-Hawthorn aquifer, respectively). For the rest of the layers (meaning those that represent the FAS, which is the focus of the study), a 5-cell neighborhood was chosen to evenly maintain the subtle changes in the hydrostratigraphic surface.

Table 3-5. Hydrogeologic units and data source(s).

Layer No.	Hydrogeologic Unit	Top/Bottom (SFWMD Filename)	Source
1	water table aquifer and Tamiami confining unit (when it exists) (Constant Head Boundary)	Topo/Aq1b	SFWMD
2	Lower Tamiami aquifer, and Upper Hawthorn confining unit	Aq1b/Aq2t	SFWMD
3	Sandstone aquifer	Aq3t/Aq3b	SFWMD
4	Mid-Hawthorn confining unit	Aq3b/Aq4t	SFWMD
5	Mid-Hawthorn aquifer	Aq4t/Aq4b	SFWMD
6	Lower Hawthorn confining unit	Aq4b/UFtop	SFWMD
7	Upper Floridan aquifer	UFtop/MCtop	USGS/SFWMD
8	Upper Floridan aquifer	UFtop/MCtop	USGS/SFWMD
9	Upper middle confining unit	MCtop/MFtop	USGS/SFWMD
10	Middle Floridan aquifer (Avon Park permeable zone)	MFtop/MFbot	USGS/SFWMD
11	Lower Middle confining unit	MFbot/LFtop	USGS/SFWMD
12	Lower Floridan aquifer (Constant Head Boundary)	LFtop/LFbot	USGS/SFWMD

In addition, the SFWMD suggested lowering the bottom of the first seven layers by 1.5 feet in order to adjust the vertical datum. Again, after that subtraction, it was sometimes necessary to make additional small changes to ensure a layer thickness of 15 feet.

Figure 3-2 shows the model domain and the location of six cross sections. Three sections: AA’, BB’ and CC’, are found along columns (depicting northwest to southeast trends), included as **Figures 3-3**, **3-4** and **3-5**, respectively. In addition, three other sections: DD’, EE’ and FF’, are found along rows (depicting southwest to northeast trends), included as **Figure**s **3-6, 3-7** and **3-8**, respectively. **Figure**s **3-9** through **3-15** show the top and bottom surfaces of model layers representing all the different aquifer units used in both versions of the model.

Layer 2 of the model represents a more complex fracture and/or karst zone unit that includes mainly the Lower Tamiami aquifer and the Upper Hawthorn confining unit. This layer accounts for the dual behavior of a (horizontally) water bearing unit and (vertically) confining units. It is assumed that Layer 2 works both as an aquifer using equivalent horizontal conductivities and as a confining layer using vertical equivalent conductivities. It is important to note that Layer 2’s components are not in any way calibration objectives for this model; this layer serves as more of a buffer zone between Layers 1 and 3. However, this layer was created to simulate the effects that those features (i.e., confinement and horizontal flow) may have on the model’s overall behavior. In the current calibration process, with very limited field information for the intermediate aquifer system (IAS) and UFA, any explained variance of the estimated potentiometric head would be a significant gain to the calibration process as a whole; however, this layer should not be used for the prediction of hydrologic responses in the Lower Tamiami aquifer (due to averaging properties in the aquifer and underlying confining unit, not to mention that said aquifer is so close to the uppermost boundary layer). The inland aquifer thickness and the hydraulic properties are distorted; however, it is not expected that the concentrations in Layer 1 will interact with those in Layer 2 in the inland areas of the model. To the west, around the shoreline, the Lower Tamiami aquifer pinches out and Layer 2 becomes mainly the Upper Hawthorn confining unit. In this zone, some concentration interactions may be expected, and the conceptual model is able to represent those transport processes.

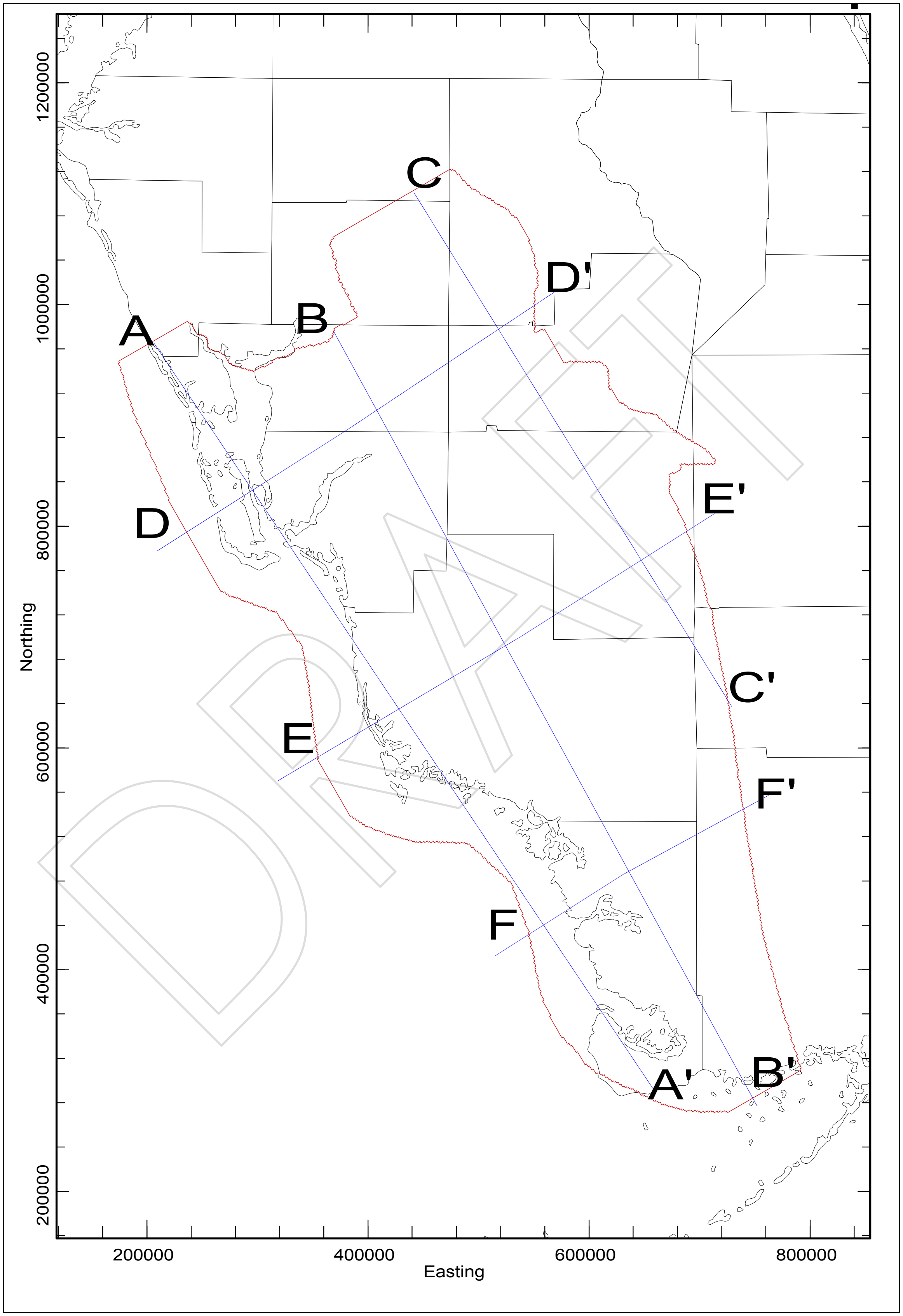

Figure 3-2. Plan view for the cross section locations.

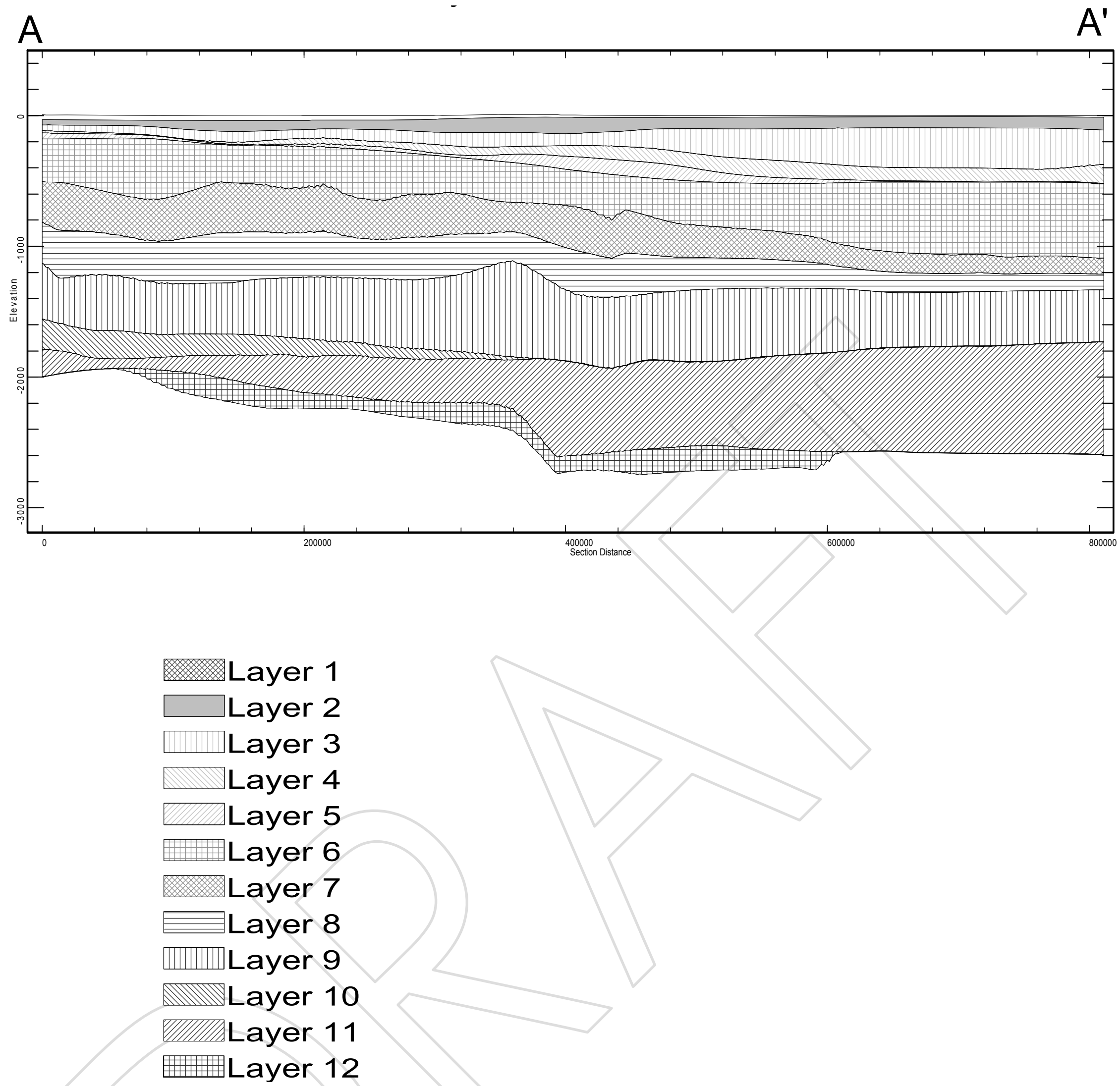

Figure 3-3. Western cross section A-A' along a grid column.

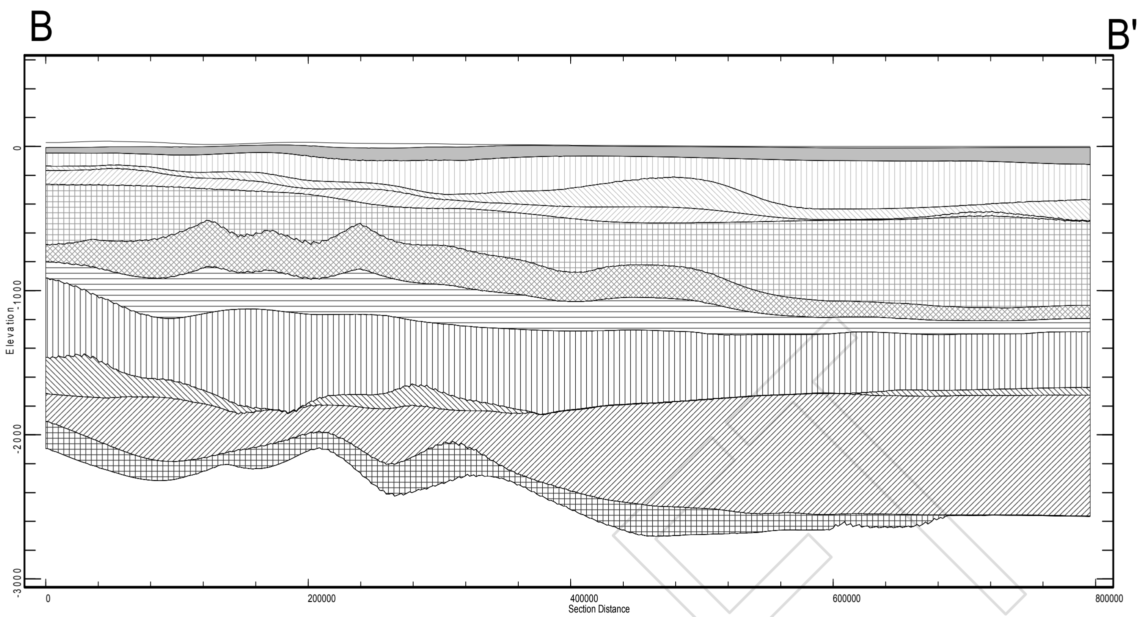

Figure 3-4. Central cross section B-B' along a grid column.

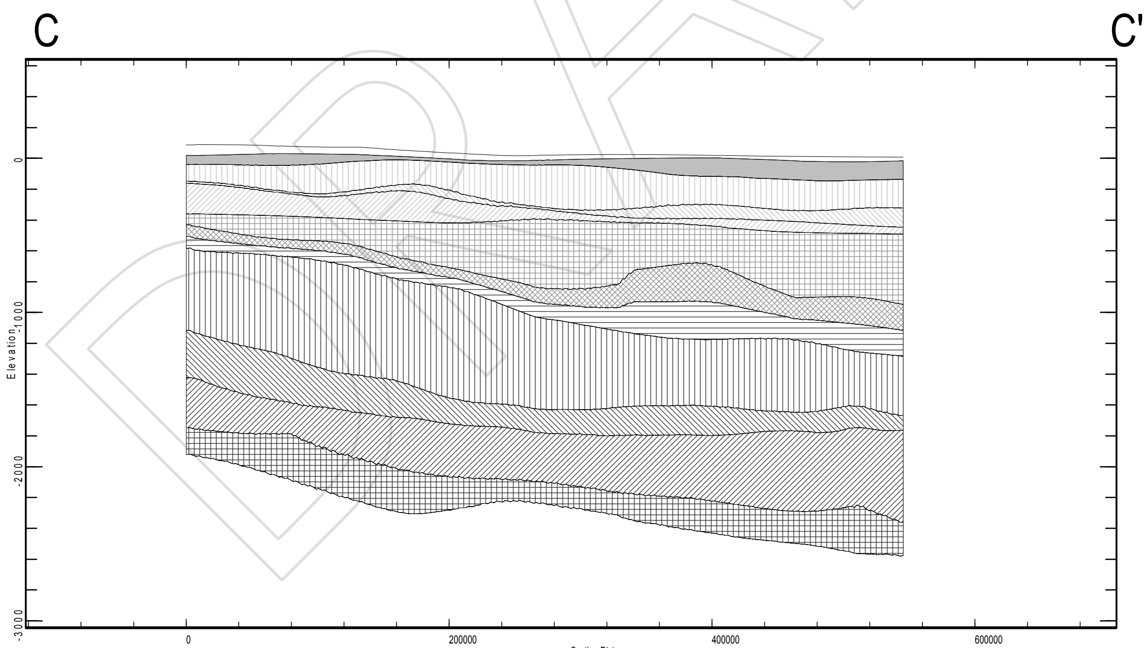

Figure 3-5. Eastern cross section C-C' along a grid column.

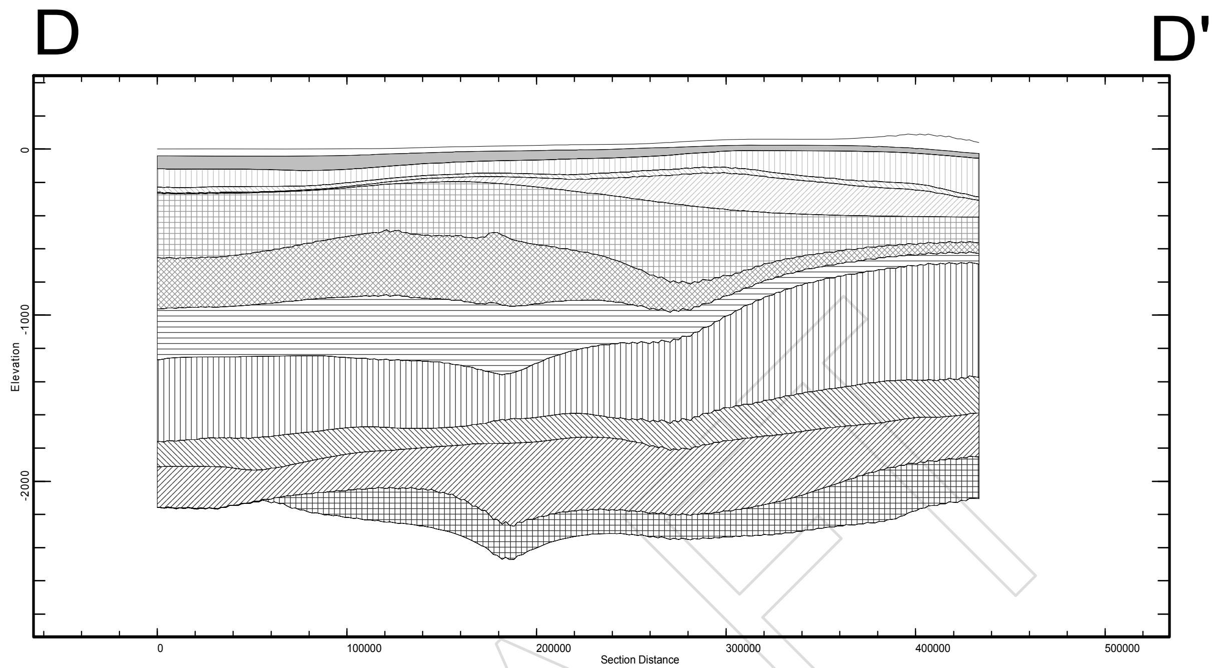

Figure 3-6. Northern cross section D-D' along a grid row.

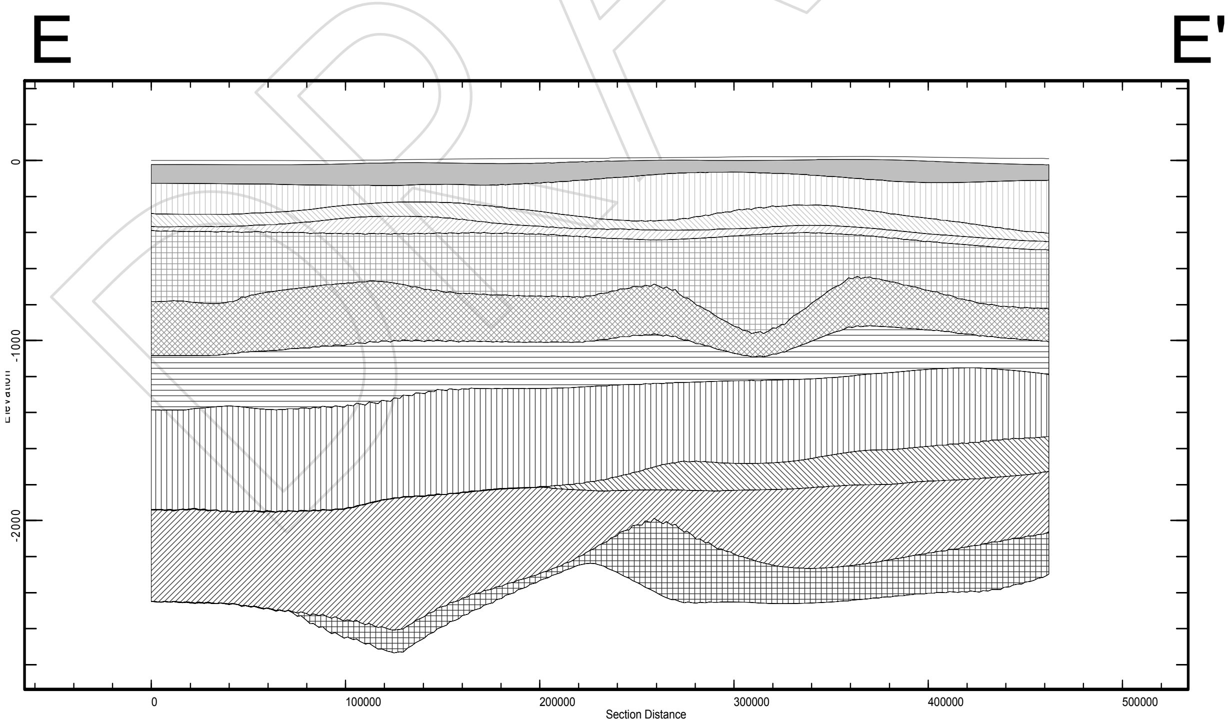

Figure 3-7. Central cross section E-E' along a grid row.

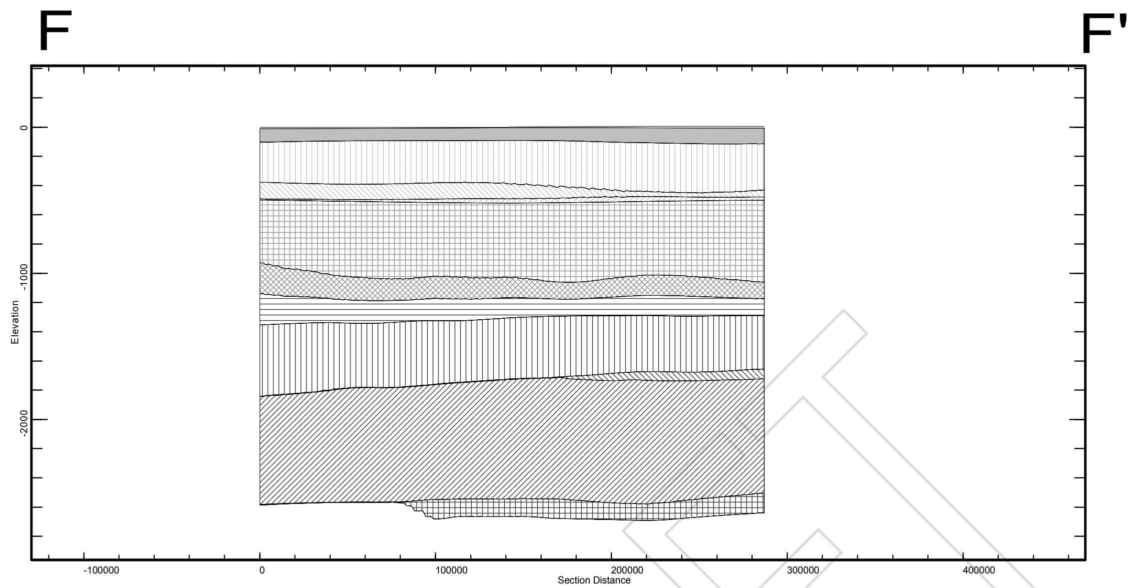

Figure 3-8. Southern cross section F-F’ along a grid row.

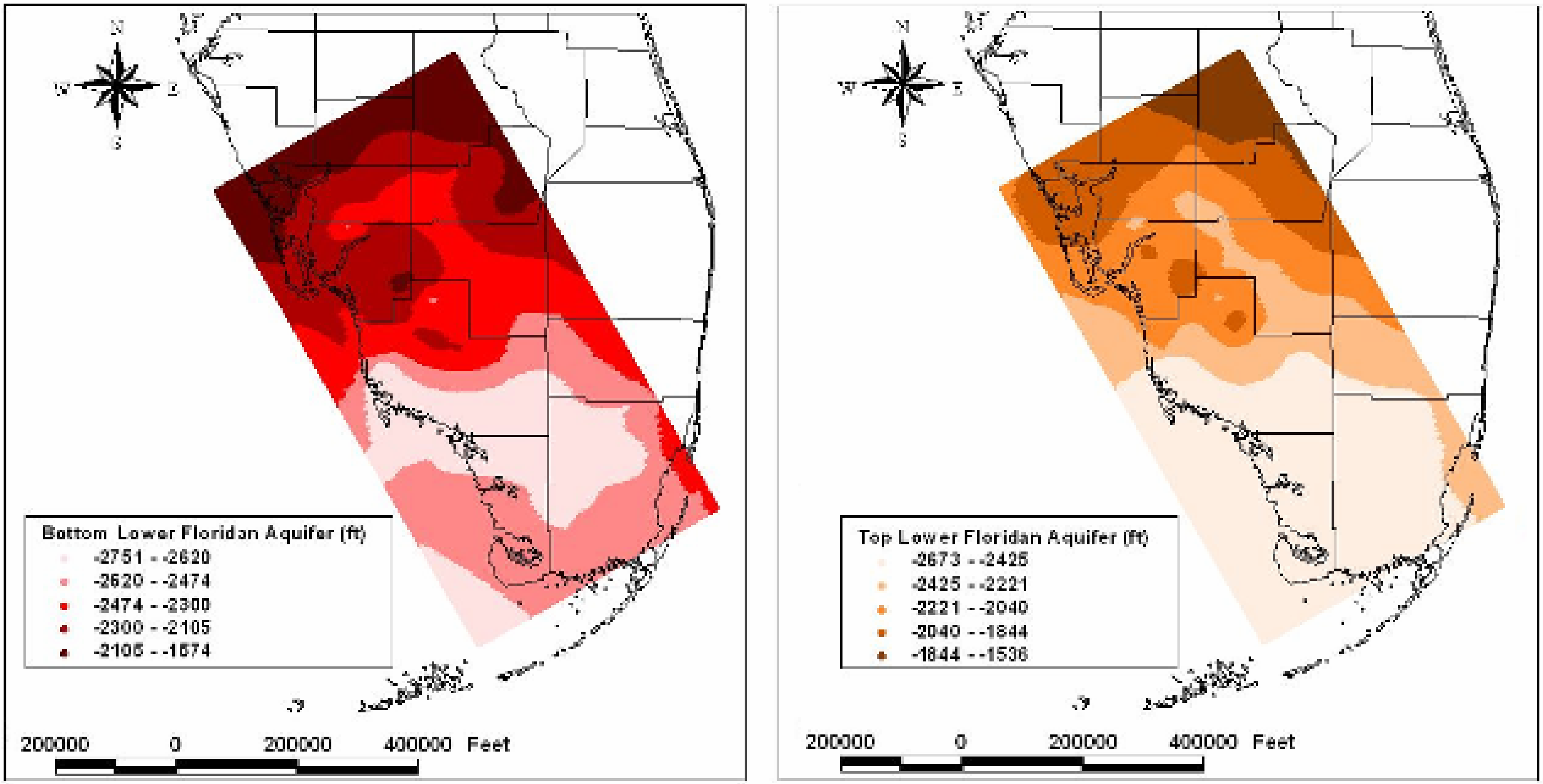

Figure 3-9. Coverages for the bottom and top of the Lower Floridan aquifer.

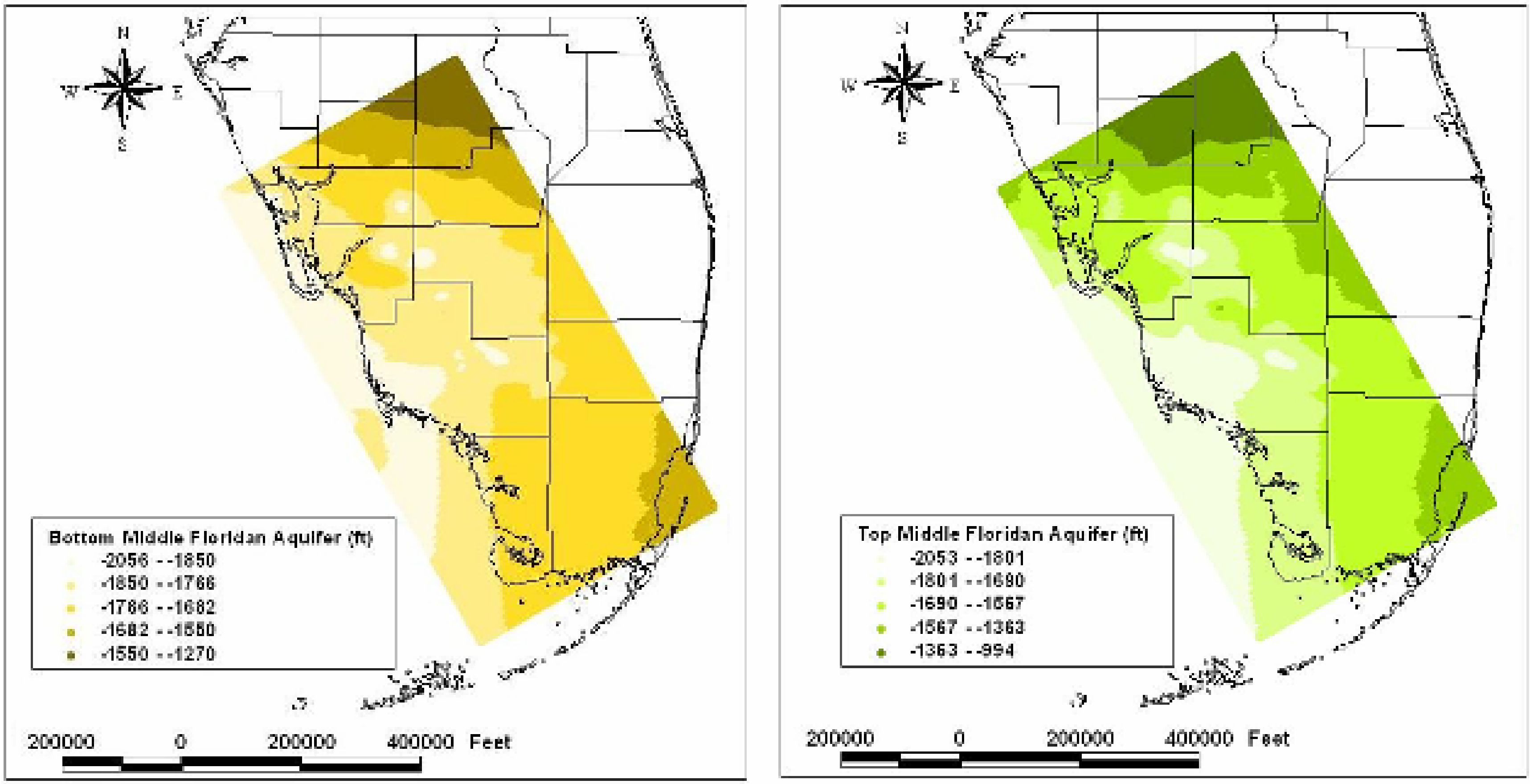

Figure 3-10. Coverages for the bottom and top of the Middle Floridan aquifer (Avon Park permeable zone).

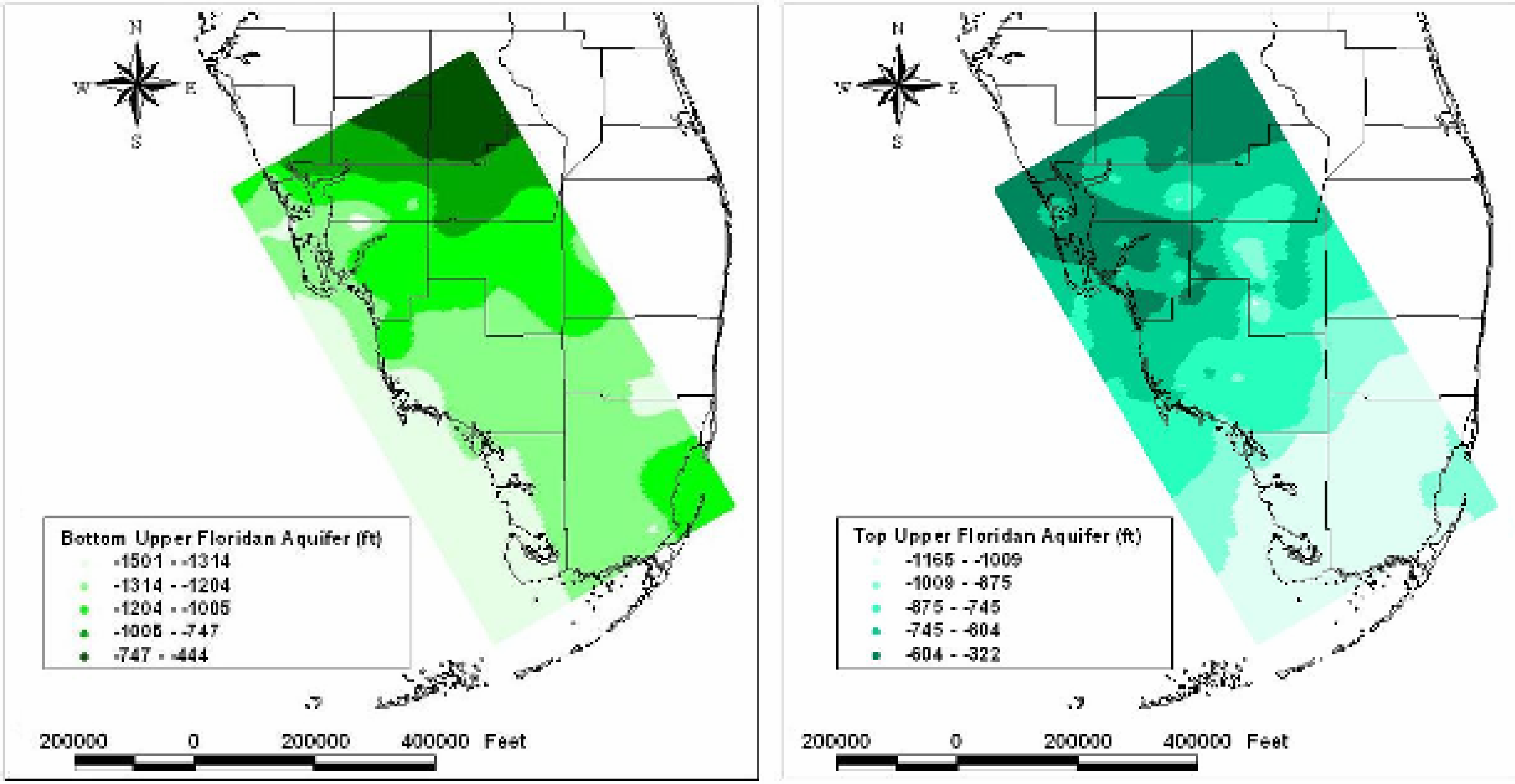

Figure 3-11. Coverages for the bottom and top of the Upper Floridan aquifer.

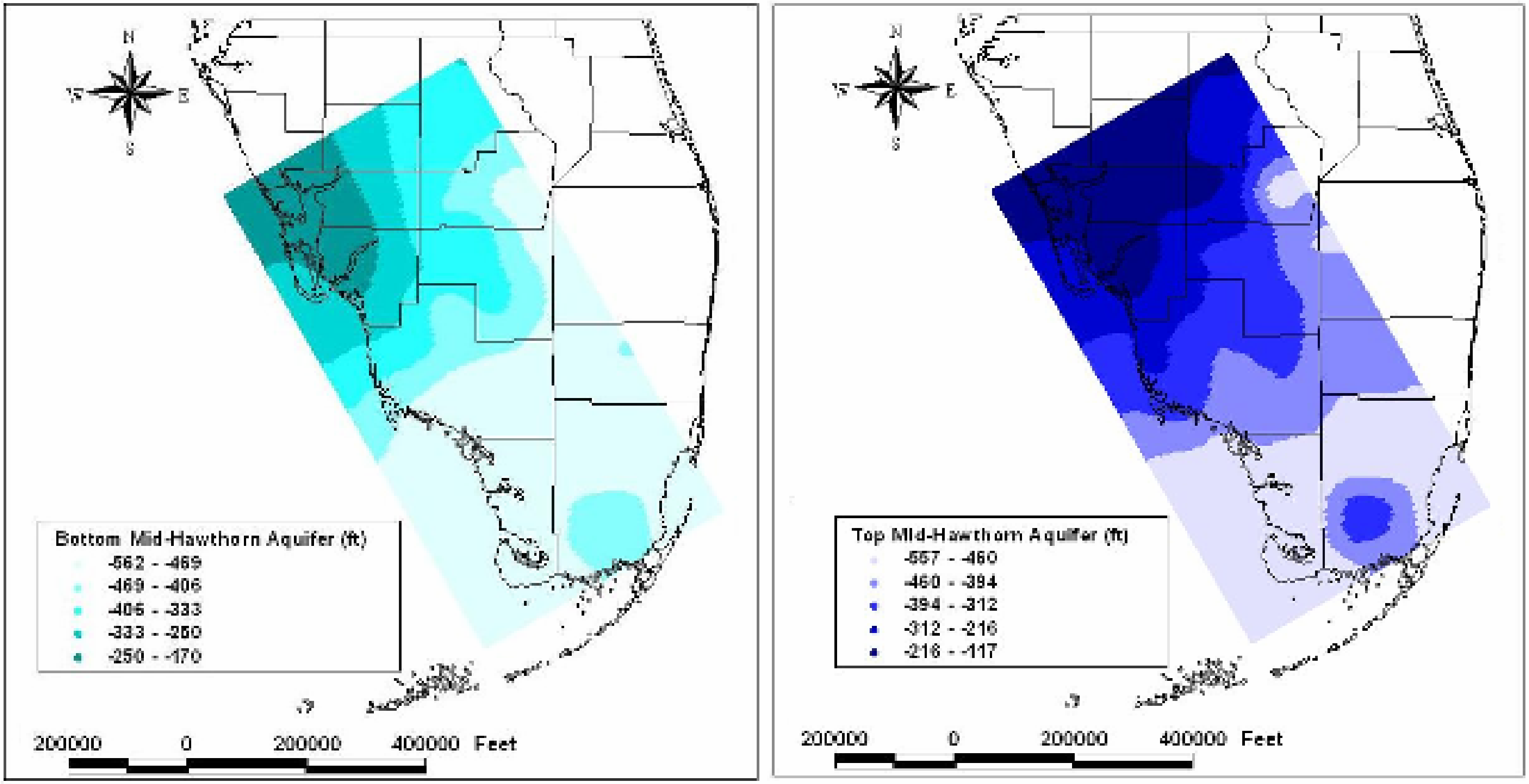

Figure 3-12. Coverages for the bottom and top of the Mid-Hawthorn aquifer.

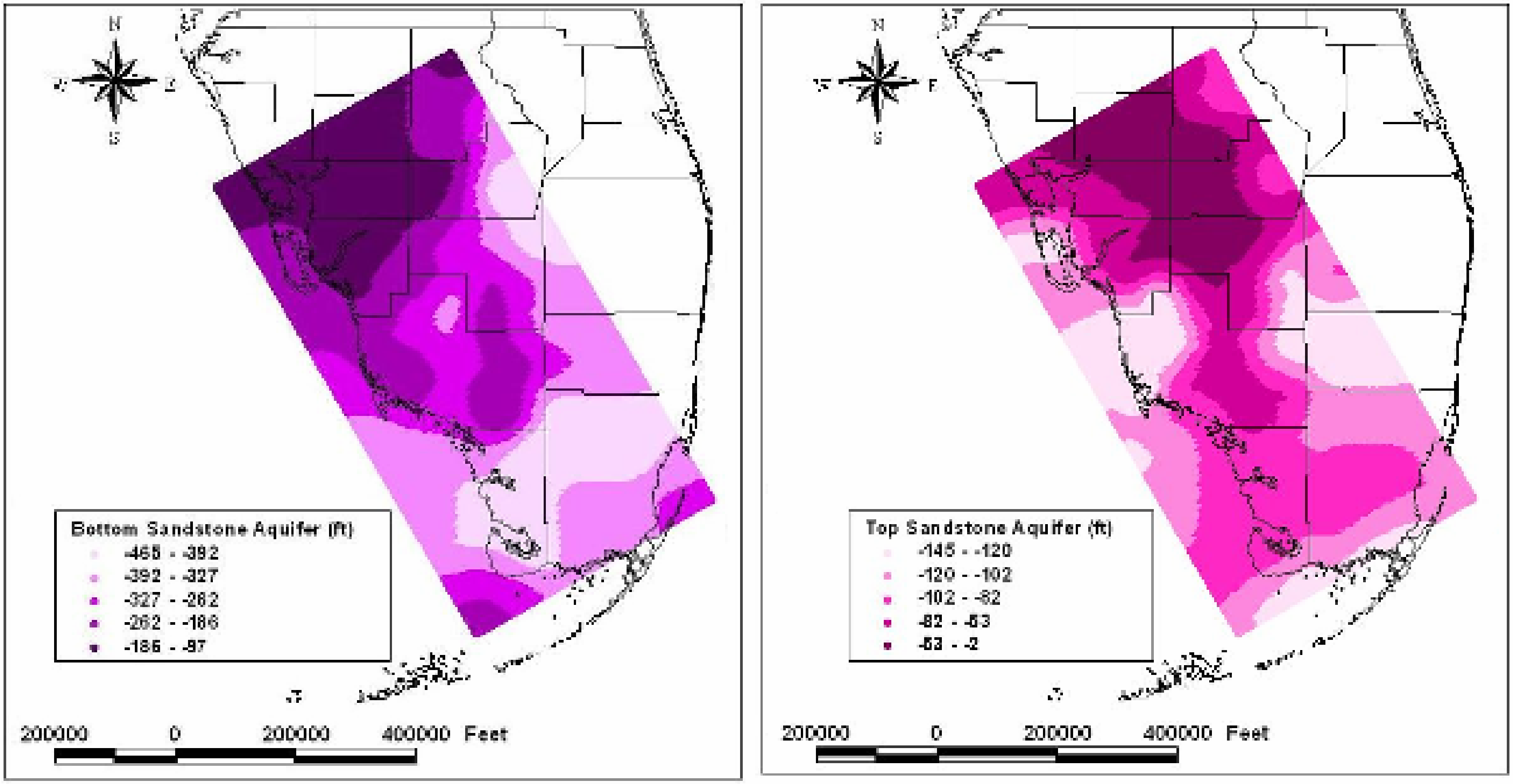

Figure 3-13. Coverages for the bottom and top of the Sandstone aquifer.

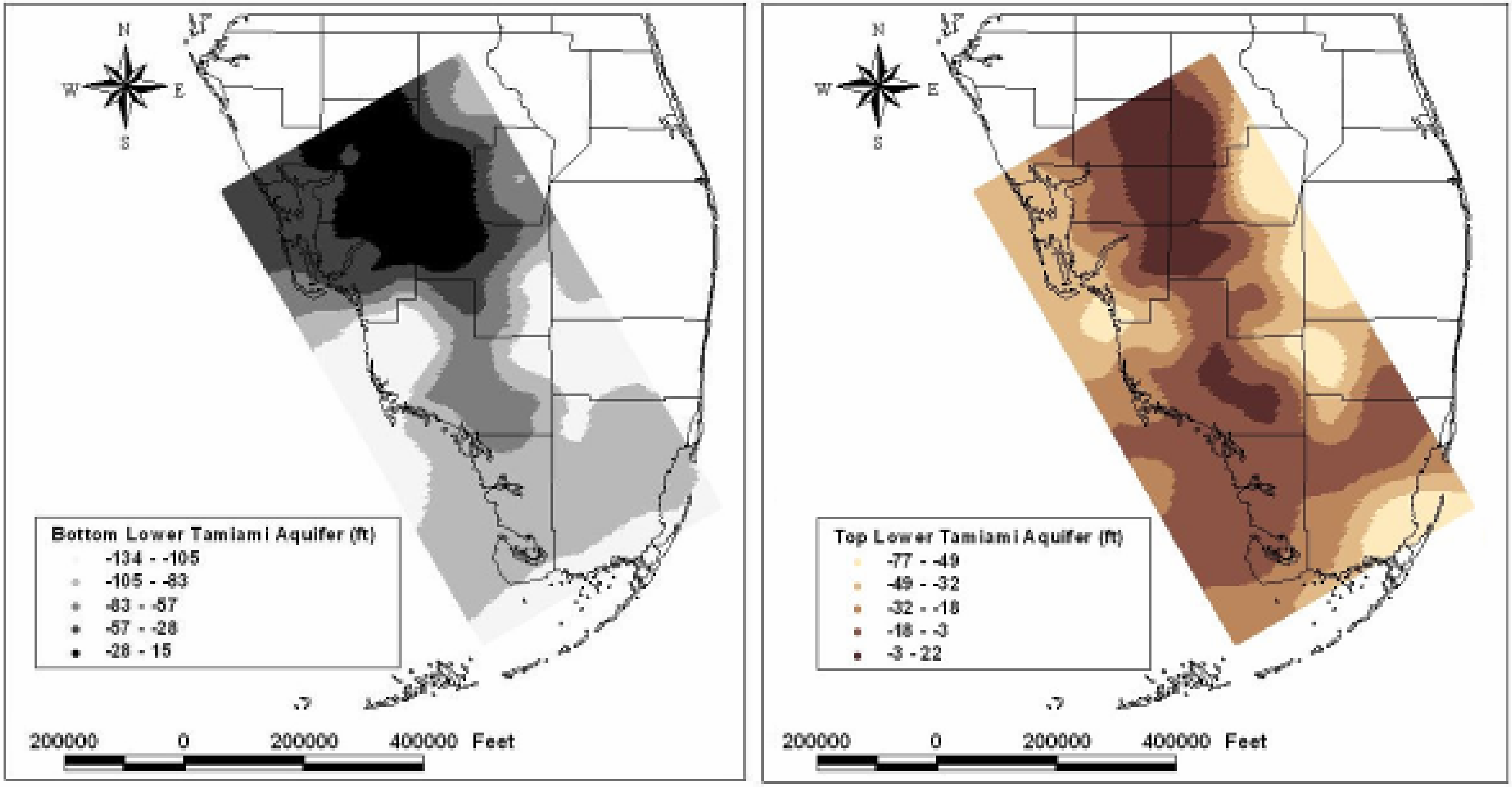

Figure 3-14. Coverages for the bottom and top of the Lower Tamiami aquifer.

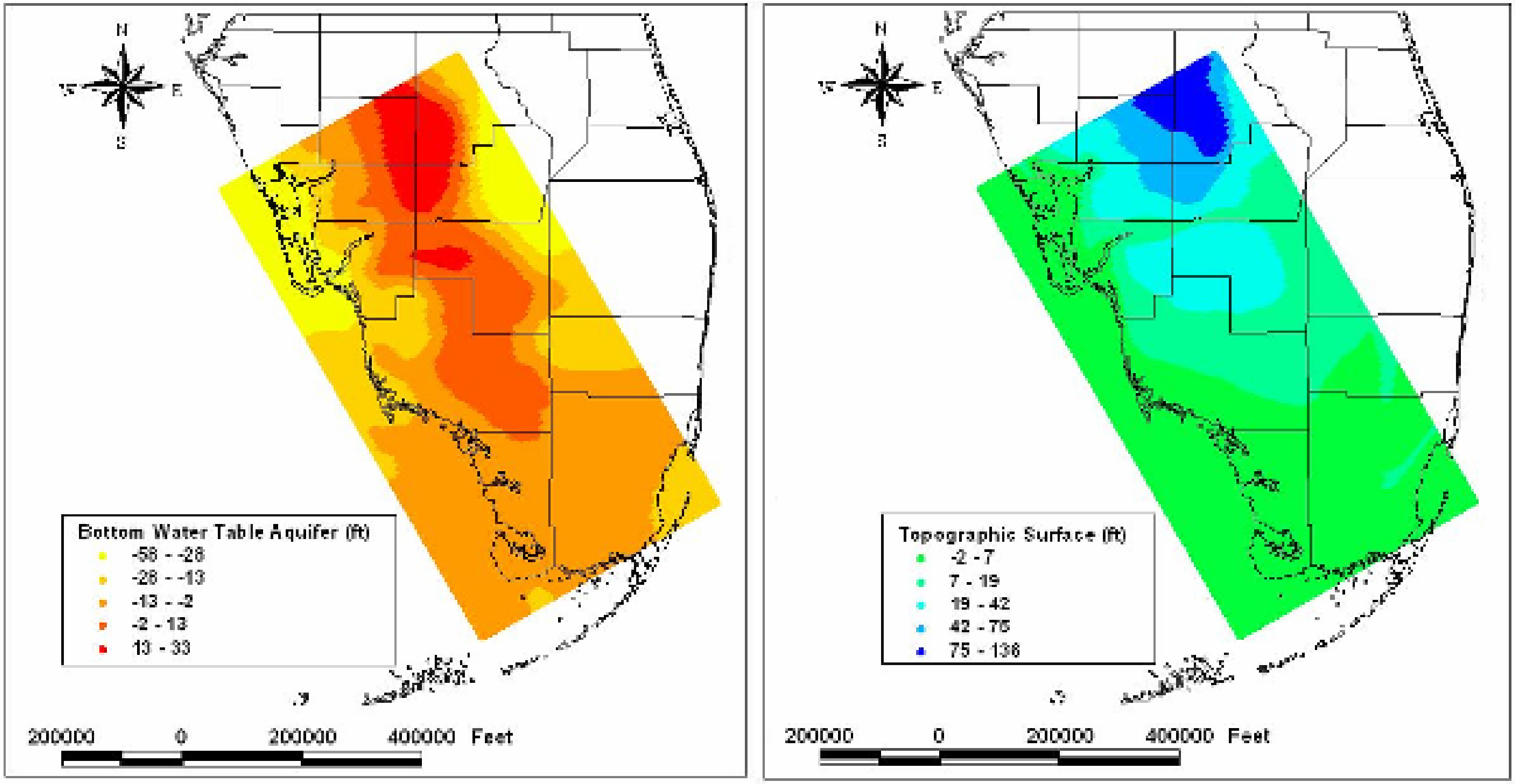

Figure 3-15. Coverages for the bottom and top of the water table aquifer.

Time Discretization

The model simulation, which runs from early 1997 to late 2001, is divided into 260 stress periods (on a weekly basis), with each time discretization including three timesteps within any given stress period. Although a weekly time scale was selected for calibration purposes, all of the data (i.e., heads/stages and flows) is set to a daily time-scale so the user can choose the stress period length. For example, to run the model on a daily basis, one only needs to change a flag in the UGEN, and then the length and number of stress periods in the UGEN main file. Transient simulation results, in terms of heads, from a number of test runs with day-long stress periods were indistinguishable from runs with week-long stress periods.

Flow and Saltwater Transport Simulator in SEAWAT-2000

Chloride concentrations are normally used to represent fluid-density/ oncentration relationships in density-dependent numerical simulations because chloride is a conservative solute (i.e., it doesn't decay). The correlation between total dissolved solids (TDS) and chloride concentrations is an approximately linear relationship in south Florida (Reese 1994). **Table 3-6** presents corresponding properties for two salinity regimes as defined by the TDS concentration in the southwestern region of the FAS (Reese 2000). In this case, it is possible to use TDS concentrations as the primary component affecting fluid densities due to its linearity.

Table 3-6. Computations of the resistivity of Floridan aquifer system formation water for two salinities as defined by dissolved-solids concentration (after Reese 2000).

Total Dissolved Solids Concentration (mg/L)	Chloride Concentration (mg/L)	Specific Conductance (Microsiemens/cm)	Resistivity (ohm-m)
10,000	5,240	14,800	0.675
35,000	18,900	48,000	208

The present scope of work does not involve the simulation of the temperature field and its effect on groundwater flow and transport. However, previous investigators have suggested that thermal circulation may have a significant effect on groundwater flow and transport in the FAS (e.g., Kohout 1965; Kohout et al. 1977). Neglecting this process may give rise to a noteworthy limitation in the current model, especially in the formulation of Layer 12.

Boundary Conditions

A conceptual groundwater flow model should embody all the important features of the flow system and identify all simplifying assumptions associated with this understanding. Mercer and Faust (1981) state that the conceptual model should consider cause and effect relationships of the modeled system to determine its behavior. Therefore, a model's boundary definition is an important consideration during its early design, since boundaries can affect flow/transport patterns and water budgets. A model boundary is the interface between the calculated model domain and the surrounding environment. This facet comes to life via mathematical equations, which represent the outer physical conditions of the model as interpreted by the modeler. In many cases, model boundaries are defined by practical objectives, especially when there are many unknowns in the surrounding environment (e.g., location of aquifer truncation).

Groundwater flow models are customarily designed to take advantage of natural and man-made flow boundaries to the greatest extent possible. In order to minimize misrepresentations during the model's formulation, the modeler should follow two principles to define the type and placement of boundaries. (1) The observed physical system should dictate the type of boundary conditions employed; and (2) where possible, model boundaries should lie great distances from main areas of interest in order to reduce any boundary effects on the simulation results. However, in some cases, the first principle is not an option, such as the case wherein the aquifer outcrops offshore. The second principle (defining an adequate distance for model boundaries) is subject to aquifer properties, hydraulic gradients and is estimated, as shown in **Figure 3-16**, which represents a possible characterization of the Gulf of Mexico (Gulf) boundary. The physical processes occurring at that boundary must be well-characterized in order to reduce uncertainty in the model results.

Discussion of Gulf Boundary Conditions

Boundary conditions representative of seawater conditions must be specified for all coastal boundaries. Native hydraulic heads and TDS concentrations are the primary state variables needed to determine boundary conditions. These parameters are used as input to the LWCFAS Model; however, measurements of these variables are very limited within the model domain.

The western boundary in the LWCFAS Model coincides with the Gulf of Mexico. In the top model layer, constant head boundaries are specified for all cells. Constant head elevations along the Gulf of Mexico (with TDS concentrations equivalent to seawater) are derived from mean sea level for the top layer. In Layers 2 and 3, constant head boundaries are specified for the western-most cells in coastal regions along the Gulf. Constant head elevations with TDS concentrations equivalent to seawater are also derived from mean sea level for these layers.

In all other model layers, including the Hawthorn Group and the underlying Floridan aquifer system (FAS), constant head and equivalent saline TDS concentrations are unknown (i.e., the mean sea level assumption and the seawater concentration assumption can not be applied directly to the deeper model boundaries). Additionally, the boundary issue becomes more complex due to the lack of measured data to support a conclusive boundary determination.

The first phase of the LWCFAS Model development focused on simulating a kind of “pre-development” condition for the establishment of reasonable boundary conditions in the Gulf of Mexico. The most significant issue with pre-development ‘calibration’ was selecting the prescribed potentiometric head and the concentrations at the boundary. Since the model boundary was located far closer to the shoreline (about 60,000 feet, see **Figure 3-16**) than the outcrop is thought to be located for the FAS, the constant head and salinity boundary that was applied on the western side resulted in some oddities in the simulated salinity distribution in areas proximal to the boundary. Furthermore, there is no physical data with which to confirm or dispute the assumed model boundary. In addition, within the interior of the model, there are scarce data for heads and salinity. Moreover, the available data for salinity is mainly for a history comprised of a lone event, the result of which is a very high uncertainty in, especially, coupled model results.

There is a reasonable “static [system] condition” related to the distribution of salinity in the FAS and IAS. The FAS (Lower Hawthorn aquifer and Upper Floridan) and the IAS (intermediate and Sandstone aquifers) account for 19 percent and 14 percent of the total water use, respectively. Most of the pumping stress comes from the surficial aquifer system (67%). FAS pumping activity is relatively small compared to the entire water budget of the aquifer (**Figure 2-7**), and a system closely resembling natural conditions was an essential model assumption along Monroe, Collier, and Lee counties, with some minor exceptions with cells neighboring production/injection wells. There is a certain point in time, during the initial model design, when one has to stop imagining the system’s most likely behavior, and recognize that there is not enough supporting data to construct a genuine coupled model. When the coupled model was initially used, unreasonable values of concentration and hydraulic conductivities were needed to maintain the head in the model domain and keep the model stable. The depiction of the Gulf boundary in **Figure 3-16** is thus hypothetical. However, a conceptual picture of the boundary must be formulated to move forward with model development. A gradually curving system was assumed in order to extend the FAS (Petuch 2008).

The authors were convinced that the assumption of a system with a static water-density distribution over time while changing in space was the best route to take (i.e., calibration without this basic assumption was full of pitfalls). As justification for this direction, the authors put forth the following approach:

- Use an alternate calibration technique assuming constant density in time but not in space,
- Extrapolate the potentiometric heads linearly to the model boundary (**Figures 2-13** and **3-16**), and
- Refine the Gulf boundary under the aforementioned assumptions and the use of current data with several pre-calibration trial-and-error simulations.

This approach used a quasi-three-dimensional steady-state simulation to refine the boundary conditions until the surface around the boundary was smooth (e.g., avoiding significant gradients – positive/negative near the boundary). The model simulation length was 10,000 days, which was long enough to produce a "steady-state" solution at the boundary area.

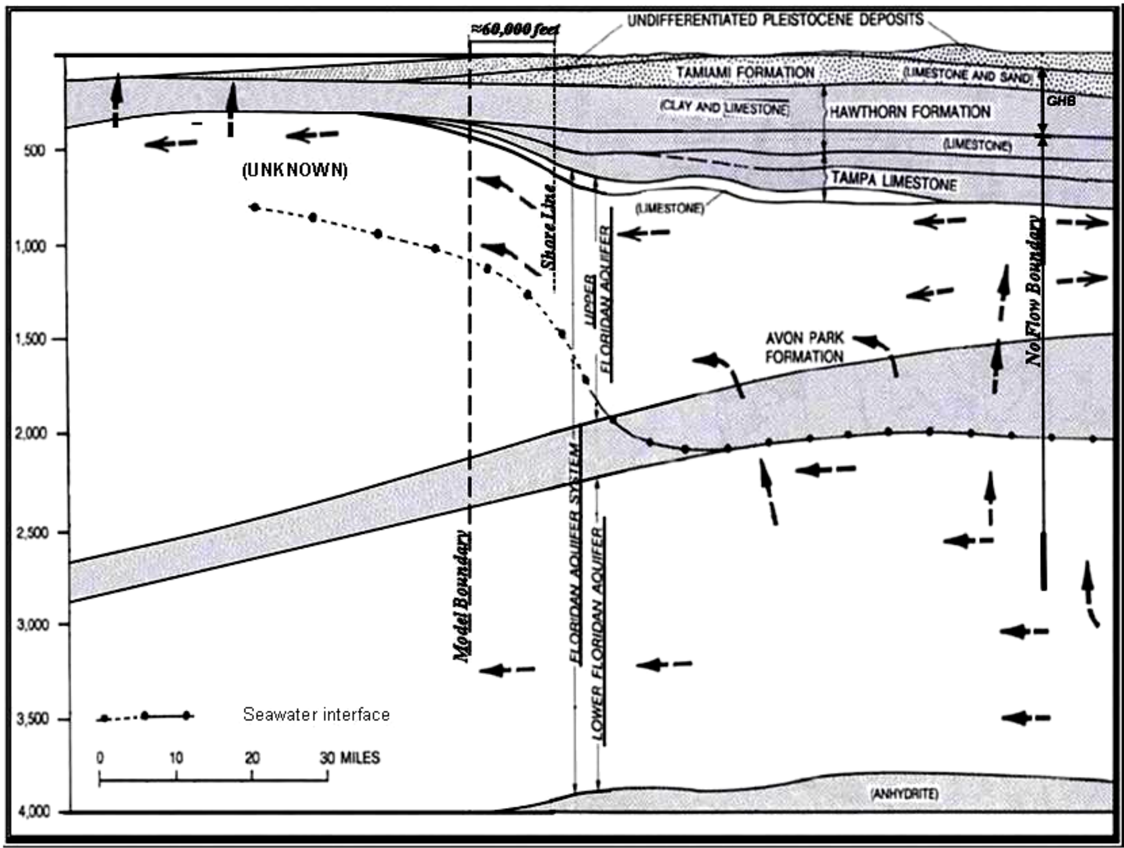

Figure 3-16. Schematic of the hypothetical Gulf boundary in an exaggerated cross section (modified from Meyer 1989).

Applied Boundary Conditions

A combination of no-flow, constant head and general-head boundaries were used in this particular model. The potentiometric heads, provided by monitoring stations and tidal stations, allowed for time-variant constant head and general-head boundaries. The TDS concentrations provided by field stations were interpolated spatially and used as constant boundaries for the simulation in Layer 1. In the case of general head boundaries along the western boundary, a concentration equal to zero was used. The constant head values in other layers were unknown.

Figure 3-17 depicts the monitoring stations from which heads or stages were assigned to constant head cells in the top layer of the surficial aquifer (Layer 1) and along the model's eastern boundaries for Layers 2 and 3. **Figure 3-18** shows the tidal stations used to define the constant head boundary along the perimeter to the west. The general-head boundary along the northern and eastern perimeters for the surficial and intermediate aquifer systems used monitoring well data. Some tidal stations were also used along the northern boundary.

The model boundaries are depicted in **Figure 3-**19 and explained as follows: The water table aquifer (in Layer 1) is represented by a constant head boundary (for all active cells) that changes over time using the appropriate observations, as depicted in **Figure 3-20**. **Figure 3-21** displays the boundary conditions for the surficial aquifer system (excluding the water table) Layers 2 and 3, the Lower Tamiami aquifer, the Upper Hawthorn confining unit, and the Sandstone aquifer. Along the Gulf, the boundary for these two layers was set via a constant head boundary that changes over time (**Figure 3-22)**, using tidal elevations (**Figure 3-20**) and the concentration of the seawater. The general-head boundary assigned to the eastern model boundary was applied using the measured elevations from the various structures and observation wells (**Figure 3-17**), with a concentration equal to zero.

As defined in MODFLOW (McDonald and Harbaugh, 1988), the boundary conductance (for each layer) is computed initially with the layer properties from the appropriate cell. This conductance was used as a calibration parameter. To the north, there is a constant head boundary based on interpolating the available data, and to the east, again, there is a no-flow boundary following the groundwater divide.

Figure 3-23 shows the boundary conditions for the FAS, not including the Boulder zone. The boundaries for Layers 4, 5 and 6 were set in a manner similar to those in the FAS (Layers 7 through 11). Along the Gulf, a constant head boundary was used for all layers within those aquifer units. To the north, there is a no-flow boundary, following the flowlines and the available data, and to the east, again, there is a no-flow boundary following the groundwater divide (see **Figure 2-13**).

Since minimal data exist to verify conditions within deeper, surficial model layers along the western boundary, it is assumed that the heads in Layers 1 through 3 are approximated by the stations depicted in **Figure 3-17**. It is assumed that the tidal variations should still have a notable effect on these model layers.

Boundary data for surficial observations was not applicable to the deeper layers. For Layers 7 and 8, which are the main focus of this study, the interpolated heads shown in **Figure 2-13** were projected toward the west (i.e., the equilibrium point), and thus a head value at the model boundary location was estimated.

To find the western boundary heads for Layers 4, 5, 6, 9, 10, and 11, the model was executed leaving the original constant head cells active until these cells reached equilibrium (at about 10,000 days). Then, the model-generated values (from the previous run) were input back into the model to refine the constant head boundary cells in some outlying cases, such that the gradient ran smoothly right up to the western border. The rationale behind this approach is that the actual boundary conditions extend far beyond the limits of the conceptualized model and that those actual boundaries are unknown (see **Figure 3-16**).

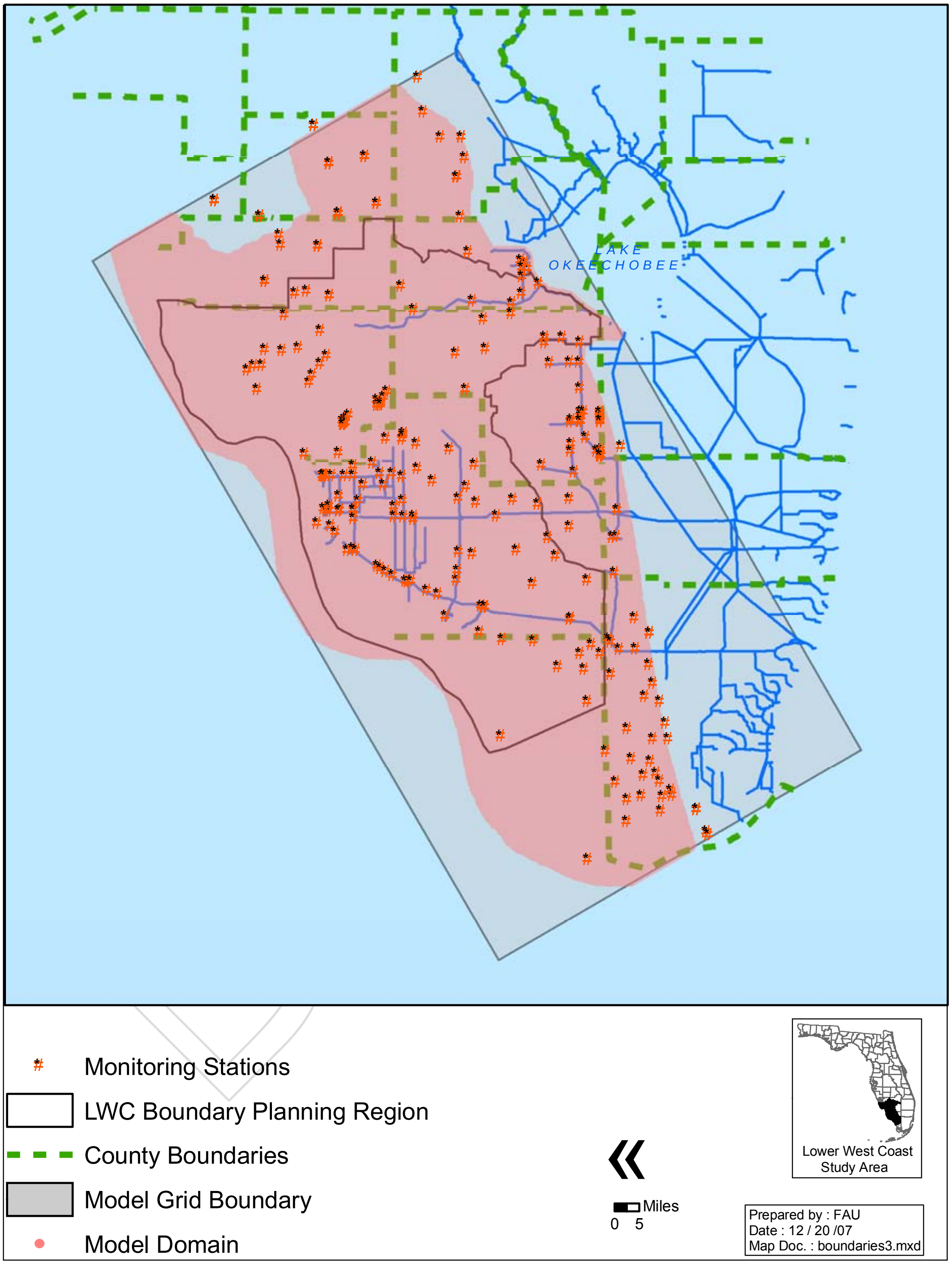

Figure 3-17. Stations used to define inland general head and constant head boundary conditions for Layers 1 through 3.

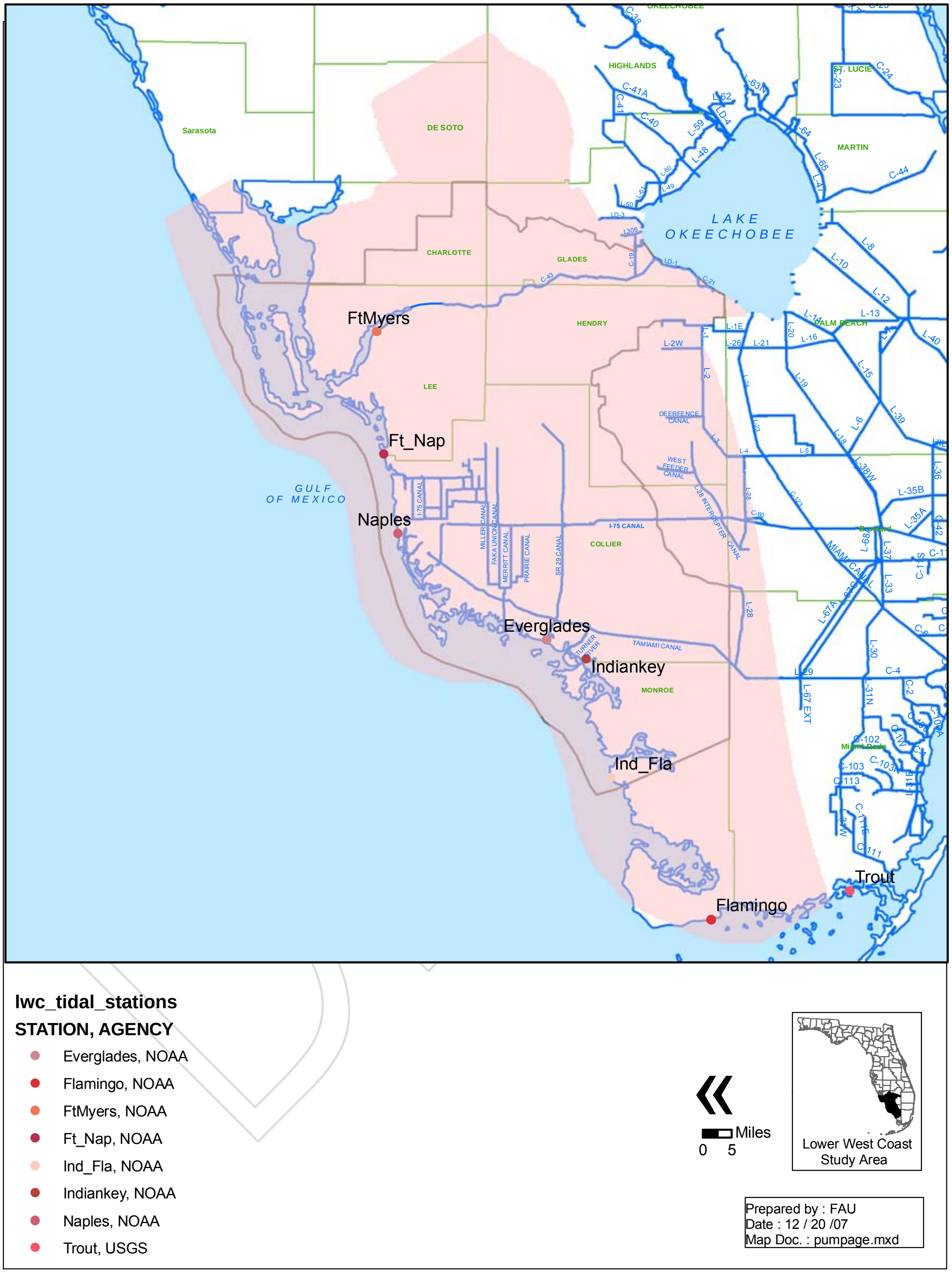

Figure 3-18. Location of tidal stations.

West / Gulf Boundary **Inland Boundary / East**

LAYER No.	HYDROGEOLOGICAL UNIT	SOURCE
1	Water Table aquifer, and Tamiami confining unit (when exists) (Constant Head Boundary)	SFWMD
2	Lower Tamiami aquifer, and Upper Hawthorn confining unit	SFWMD
3	Sandstone aquifer	SFWMD
4	Mid-Hawthorn confining unit	SFWMD
5	Mid-Hawthorn aquifer	SFWMD
6	Lower Hawthorn confining unit	SFWMD
7	Upper Floridan aquifer	USGS / SFWMD
8	Upper Floridan aquifer	USGS / SFWMD
9	Upper middle confining unit	USGS / SFWMD
10	Middle Floridan aquifer (Avon Park permeable zone)	USGS / SFWMD
11	Lower Middle confining unit	USGS / SFWMD
12	Lower Floridan aquifer - 1st permeable zone (Constant Head Boundary)	USGS / SFWMD

Constant Head Boundary
General Head Boundary
No Flow Boundary
Layers of Focus for Project

Figure 3-19. Representation of layer boundaries**.**

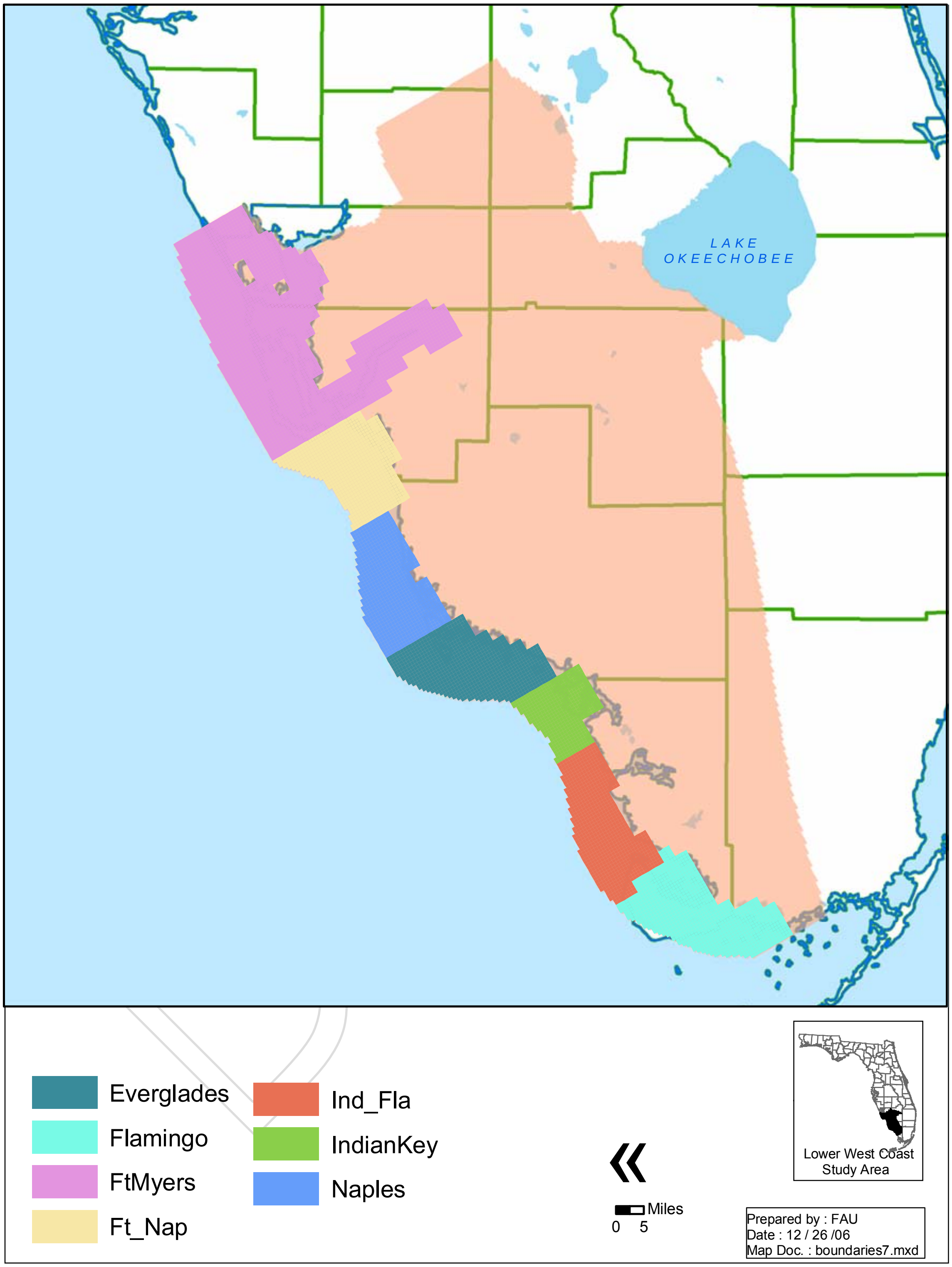

Figure 3-20. Stations used to define in costal areas general head and constant head boundary conditions for Layers 1 through 3.

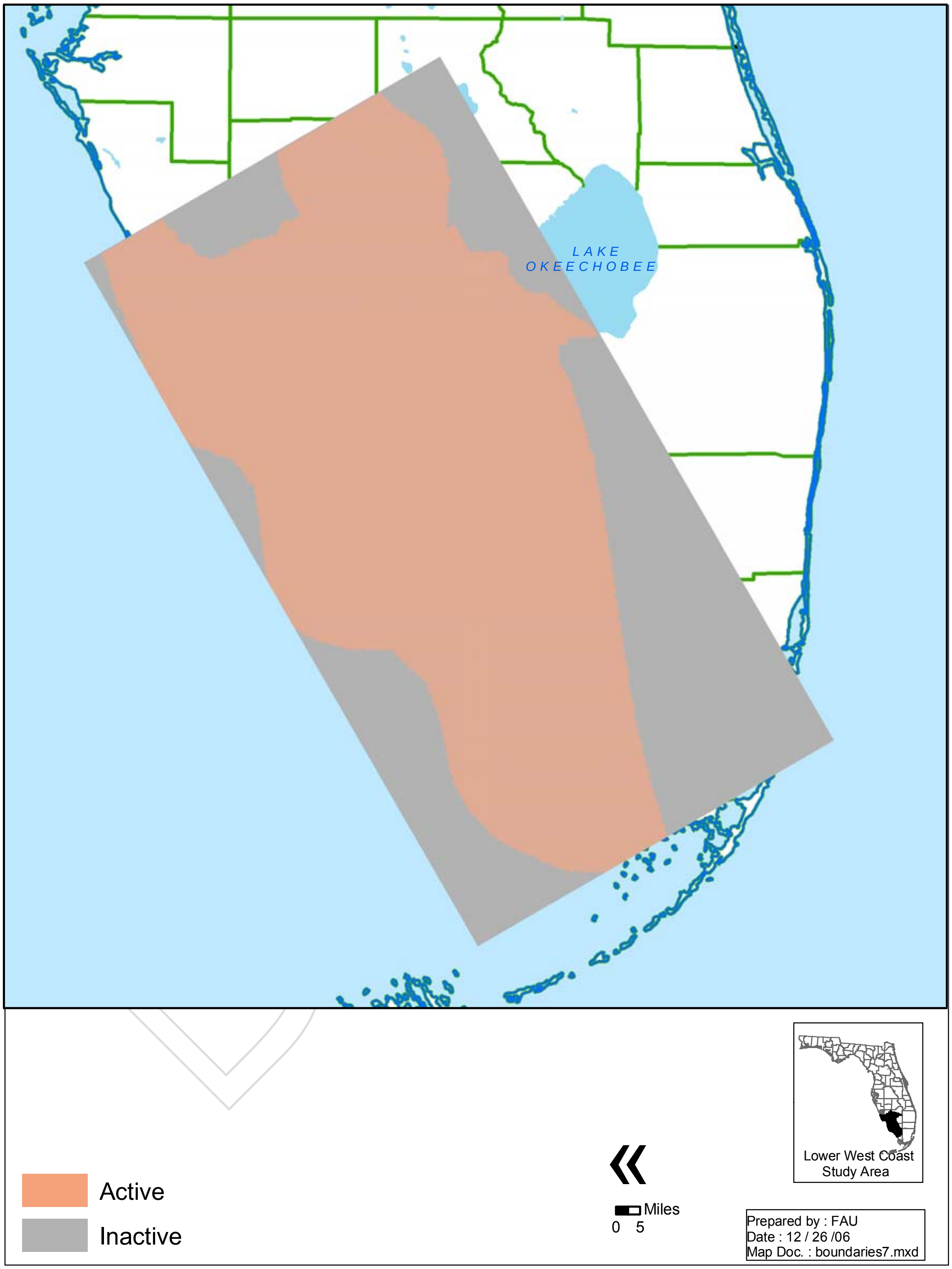

Figure 3-21. Constant head boundary conditions for Layer 1, the water table aquifer (within the surficial aquifer system).

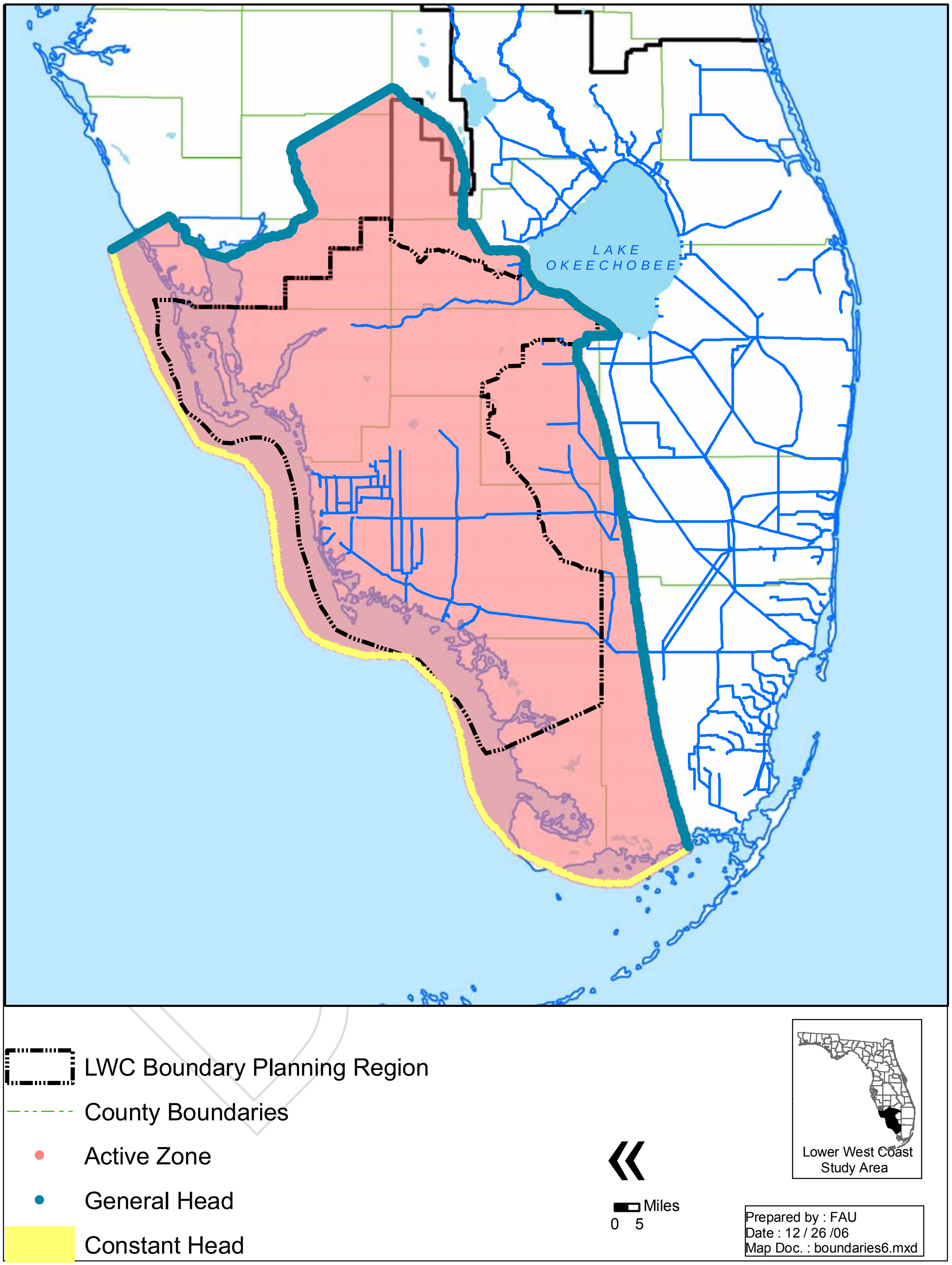

Figure 3-22. Boundary conditions for Layers 2 and 3.

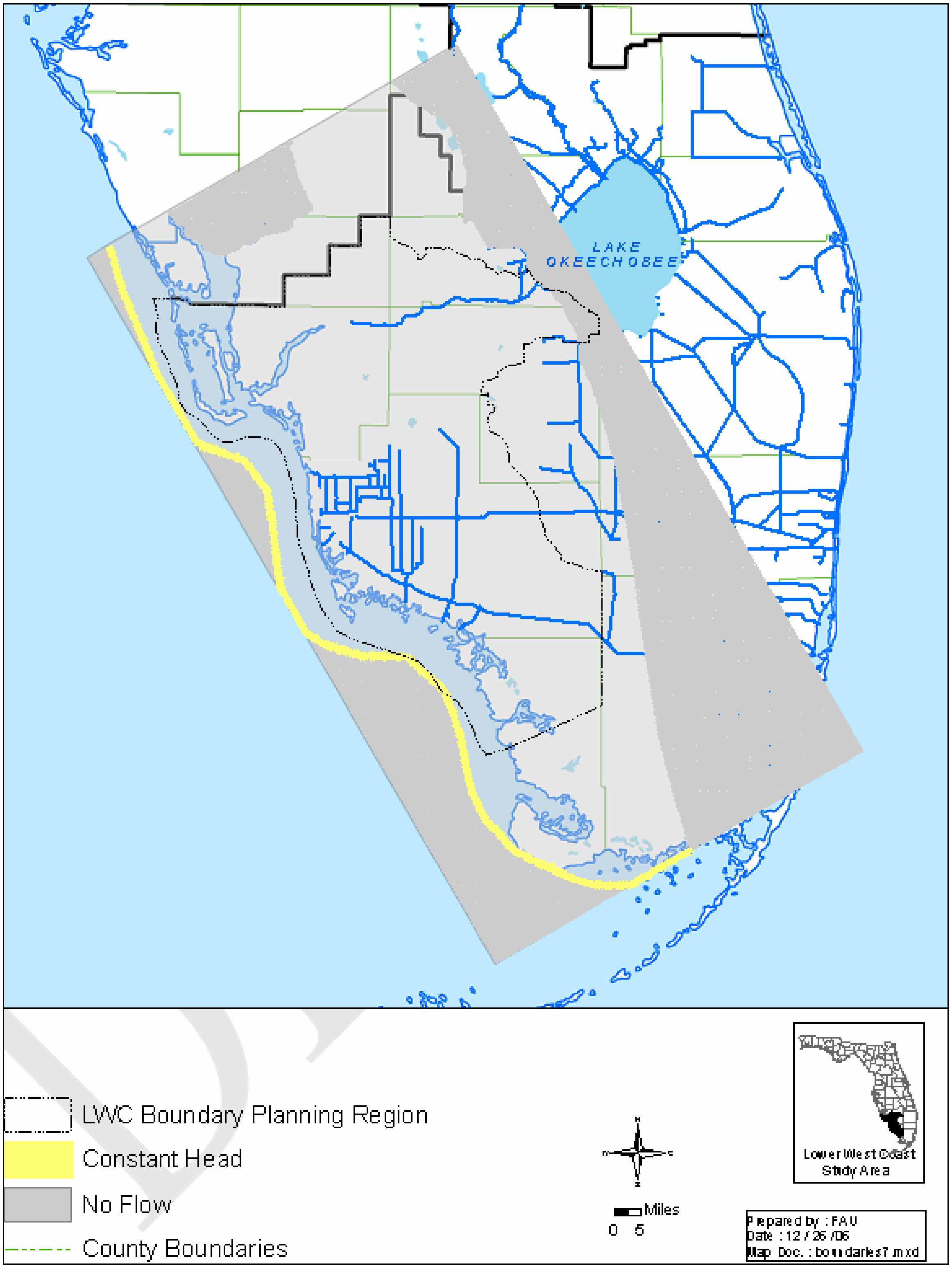

Figure 3-23. Boundary conditions for Layers 4 through 11.

A known value was assumed for the boundary condition in Layer 12. The Lower Floridan aquifer (i.e., Layer 12) has a head distribution based on salinity and temperature. The Boulder zone within the LFA has a poorly understood heterogeneous character; highly permeable potential injection zones occur at irregular vertical and lateral intervals. The water in the Boulder zone is compositionally similar to that of seawater, if not even higher in salinity (Maliva and Walker 1998).

The positions of Layer 12's boundaries were picked using lithological and geophysical characteristics of the formations in southwestern Florida. Since the understanding of the lithology is still incomplete, the boundary locations should be viewed only as educated approximations. The Boulder zone, like all of the FAS, is not one big massive horizon, but multiple thin horizons. This is probably particularly true of the LWC Planning Area.

The methodology applied to Layer 12 was proposed by Richardson (2006) for use in the Boulder zone. The top of Layer 12 is the first permeable zone in the LFA. The calculation method used to estimate the difference in density is based upon deviations from standard temperature (see **Figure 3-24**). The temperatures considered in the calculations were based on native water values prior to well injection. It would be very difficult to map current conditions (Boulder zone included) because the only data available is from the injection wells themselves, and consequently, the data are only representative of native and injected water mixed together. Additionally, the effects of pressurization (due to years of injection) are not even considered. Nonetheless, these aforementioned effects are localized to the vicinity of these wells.

It is very challenging to use the information (stated in the previous paragraph) to compute the current potentiometric head (an action which ends up providing Layer 12's constant head boundary). Thus, temperature-derived head estimates (as found in **Figure 3-25**) were applied to achieve realistic and representative pre-development conditions. Absolute verification of this hypothesis can be determined upon receipt of actual data from newly constructed wells in the Boulder zone that have not been influenced by injection wells (Richardson 2006).

The methodology applied by Richardson (2007) is presented in **Appendix B**: the main assumptions follow:

1. A constant TDS of 37,500 ppm was selected;
2. In the absence of temperature effects, the Boulder zone head distribution would be constant and equal to zero;
3. The specific weight at standard temperature (4°C) is 64.07 lb/ft^3; and
4. The reference depth is estimated as nearing the top of the Boulder zone (i.e., the top altitude of the Boulder zone ranges between 2,900 feet and 3,100 feet below sea level).

Boundary Discussion

This particular approach in defining boundary conditions used readily available information to build a conceptual model with practical, yet convincing results. This approach does put limitations on the applicability of the model and its results. However, the areas involving the “inferred boundary conditions” are more than 60,000 feet away from the shoreline, such that, in the end, this inference does not have a significant effect on the regions of greatest modeling interest, when considering the short-term future (e.g., the next 30 years).

A more technically sound application of this idea would be to:

5. Extend the active model to its projected outcrop area with permeabilities more representative of on-shore trends in the field data (the UFA outcrop is probably 200 miles to the west in the Gulf of Mexico);
6. Apply a general-head boundary at the expected outcrop, using the conductance term to adjust for reduced permeability due to overlapping fine sediments; and
7. Determine through field investigation the vertical conductance for the confining unit(s)
8. Determine through field investigation the outcrop for all the aquifers and confining units

However, this solution is not practical for the Gulf scenario because the shallow waters of the straits of west Florida occur farther away from the shoreline in southwest Florida, since the slope of the bathymetry is very gentle and gradual, as depicted in **Figure 2-2** If these gradual slopes are linked to a greater thickness of overlapping low permeability sediments, water may be channeled (in greatest proportion) toward the West, where it could find an easier escape route at the outcropping as illustrated in **Figure 3-16**. Assuming that the above information became available, the grid would need to be extended too far to the west. That model domain would be impractical for a finite-difference approach.

As a final note, the general-head boundary conditions were applied to the deeper northern and eastern layers of the model. They were later removed because they were not playing any important role in determining the neighboring potentiometric heads, and no role at all in the actual study area. In addition, there was no significant information available for the head and concentration boundaries.

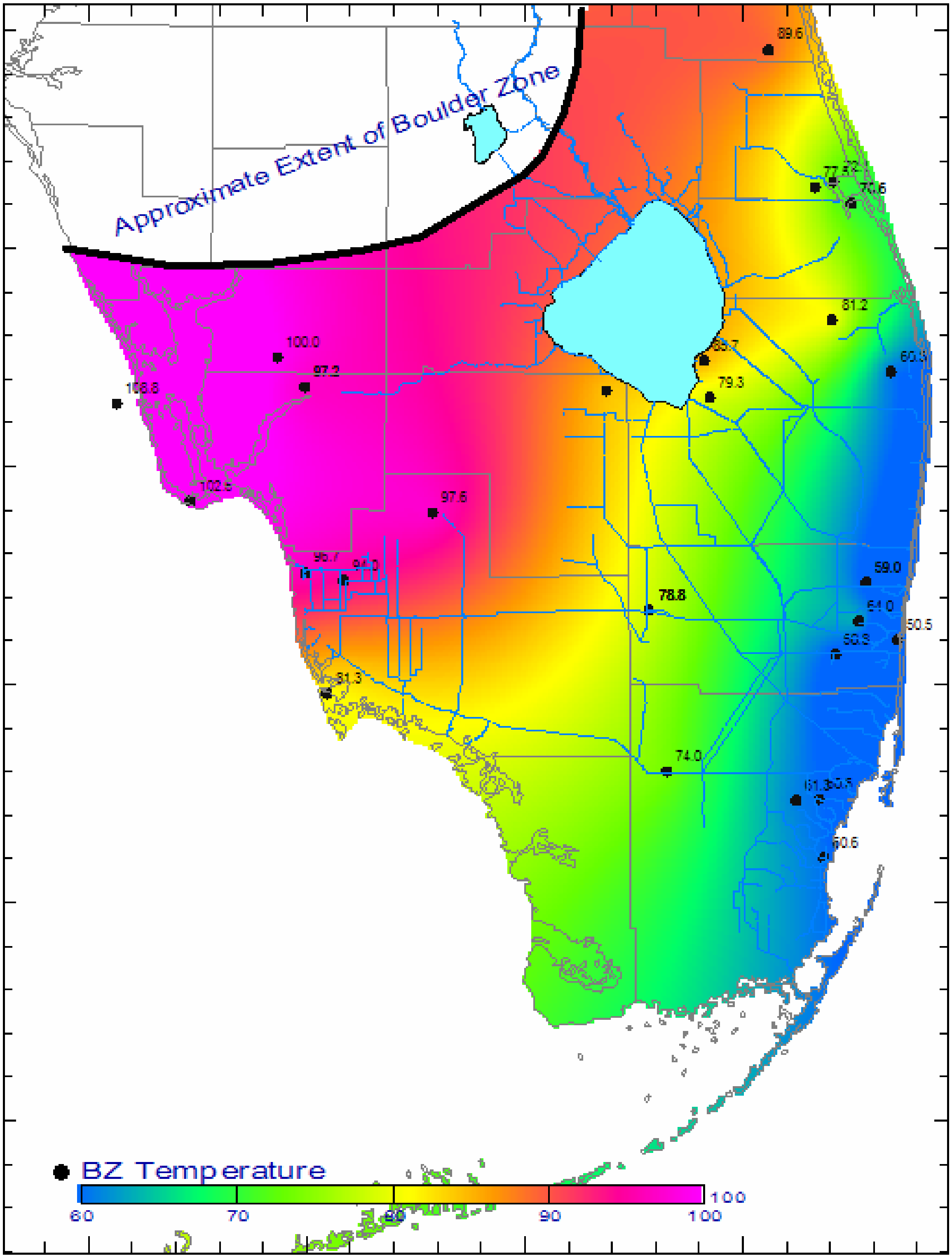

Figure 3-24. Observed pre-development Boulder zone temperature in degrees (F°) (After Richardson 2006).

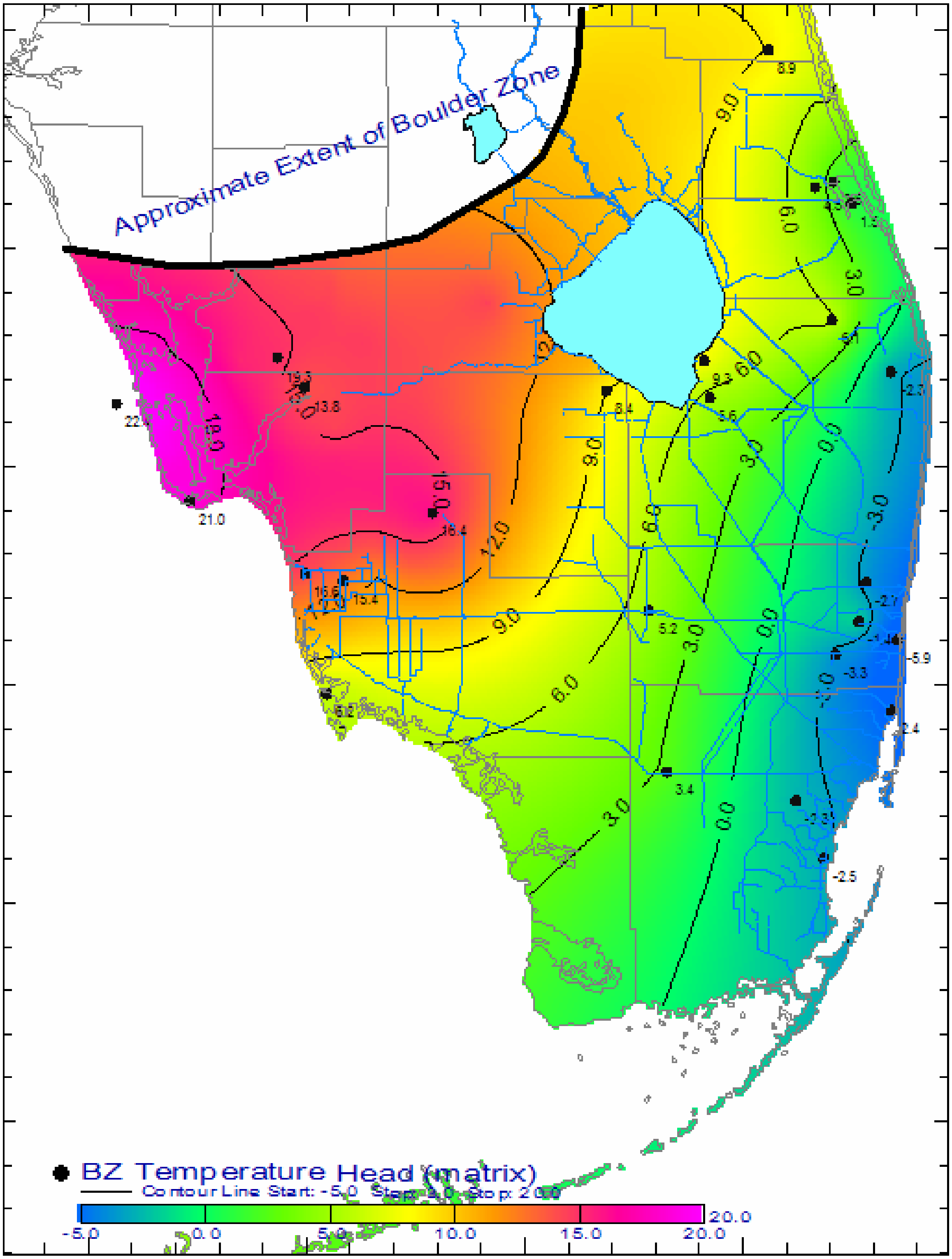

Figure 3-25. Potentiometric head [feet NGVD] value distribution of the Boulder zone estimated as a result of temperature-induced density differential (After Richardson 2006).

Summary of Initial System Properties

The LWCFAS Model simulates the flow pattern in a density-dependent domain from Sarasota County to the south end of the Florida Peninsula. The following part of the report contains a compilation of the data used in the model. Data were mainly obtained from the SFWMD, Southwest Florida Water Management District (SWFWMD), NOAA, Lee County Utilities and the USGS. GIS shape files of all data collected were created to show locations of the wells.

The data from the SFWMD contained information pertaining to water levels, chlorides, pumpage and hydrogeologic units. Data were accessed through the hydrologic database, DBHYDRO and compiled by the SFWMD (Rickabus 2005 and 2007). Other SFWMD staff (Richardson and Bennett 2005 and 2006) provided data for observation wells in the FAS. The data provided were for wells in Hendry, Lee, Monroe, Collier, Glades and Charlotte counties. SWFWMD provided water levels, chlorides, pumpage and hydrogeologic data for Charlotte and Sarasota counties. Lee County Utilities provided production well data from within the county; some chloride data were also provided for a few of the wells. Data from the USGS website included water levels and chloride levels for counties within the model domain.

The LWCFAS Model used tidal data to define the boundary condition for the western part of the model domain. Data from NOAA contained historical tidal elevations measured per day for five cities: Everglades City, Indian Key, Flamingo, Naples and Fort Myers (see **Figure 3-20**).

Monitoring Data

Head data

The monitoring data were obtained primarily from SFWMD, SWFWMD and the USGS. Initially there were 64 wells from the USGS, 127 wells from the SWFWMD and about 1,400 wells from the SFWMD. QA/QC analyses were performed to remove data that was deemed unsuitable or outside of the model domain; after the QA/QC, the total number of monitor wells was reduced to 61 wells, some of them with continuous records and some with enough records that a trend could be identified. It is important to point out how poorly distributed the monitor wells are; most are in Layers 2 and 3 and only a handful (i.e., 12 wells) are in the FAS. In addition, several of the wells are found in clusters. **Appendix C** shows the characteristics of the monitor wells used in the calibration, while **Figure 3-26** shows their location.

TDS and Chloride Data

Chloride data were primarily obtained from the SFWMD, SWFWMD and USGS. The location of wells with available TDS or chloride concentration data used in the LWCFAS Model is shown on **Figure 3-27**. Most of the chloride data points have only one record in history. **Table 3-7** describes the distribution of chloride wells used in the model per aquifer system.

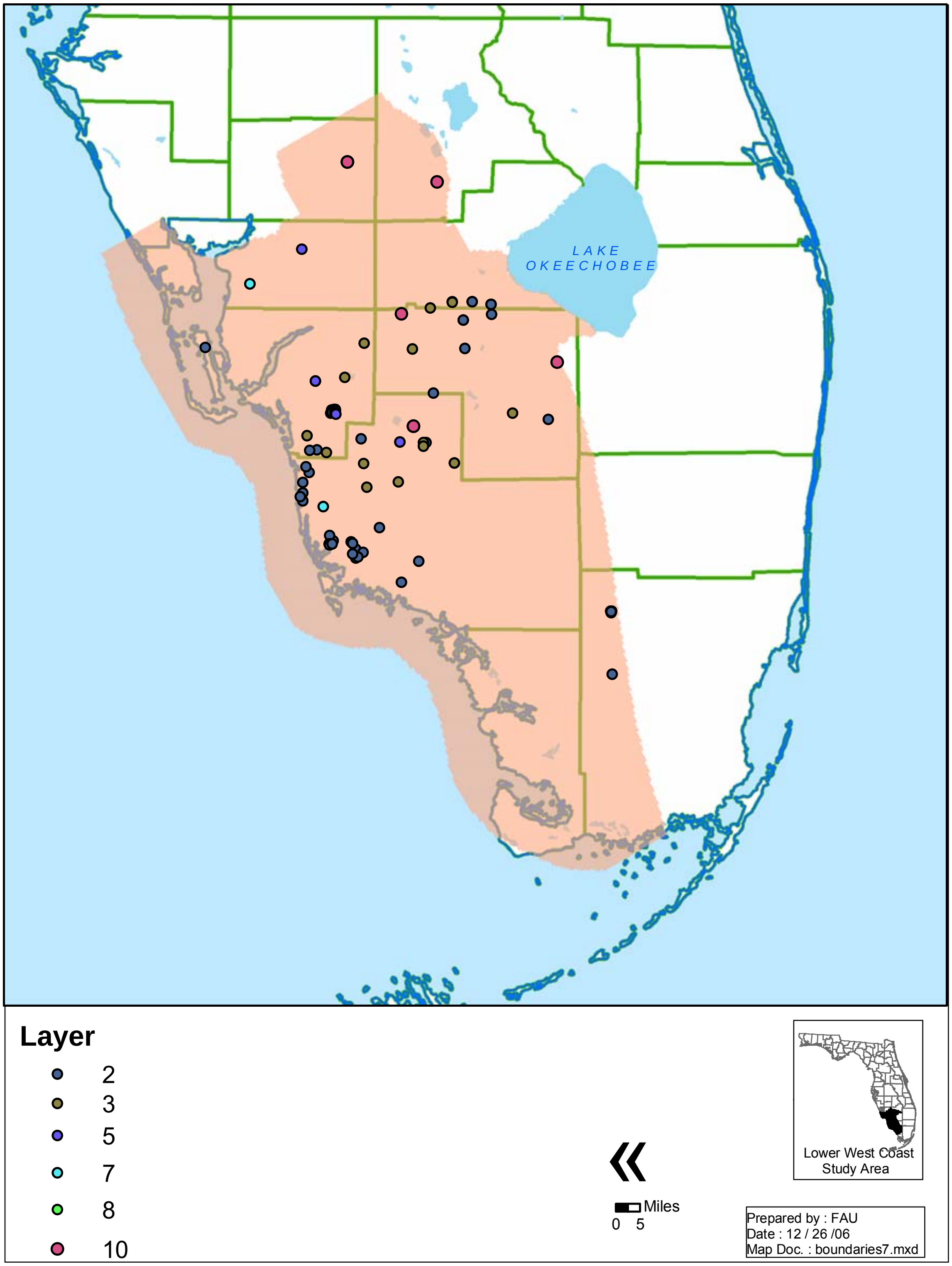

Figure 3-26. Location of monitor wells used in the LWCFAS Model.

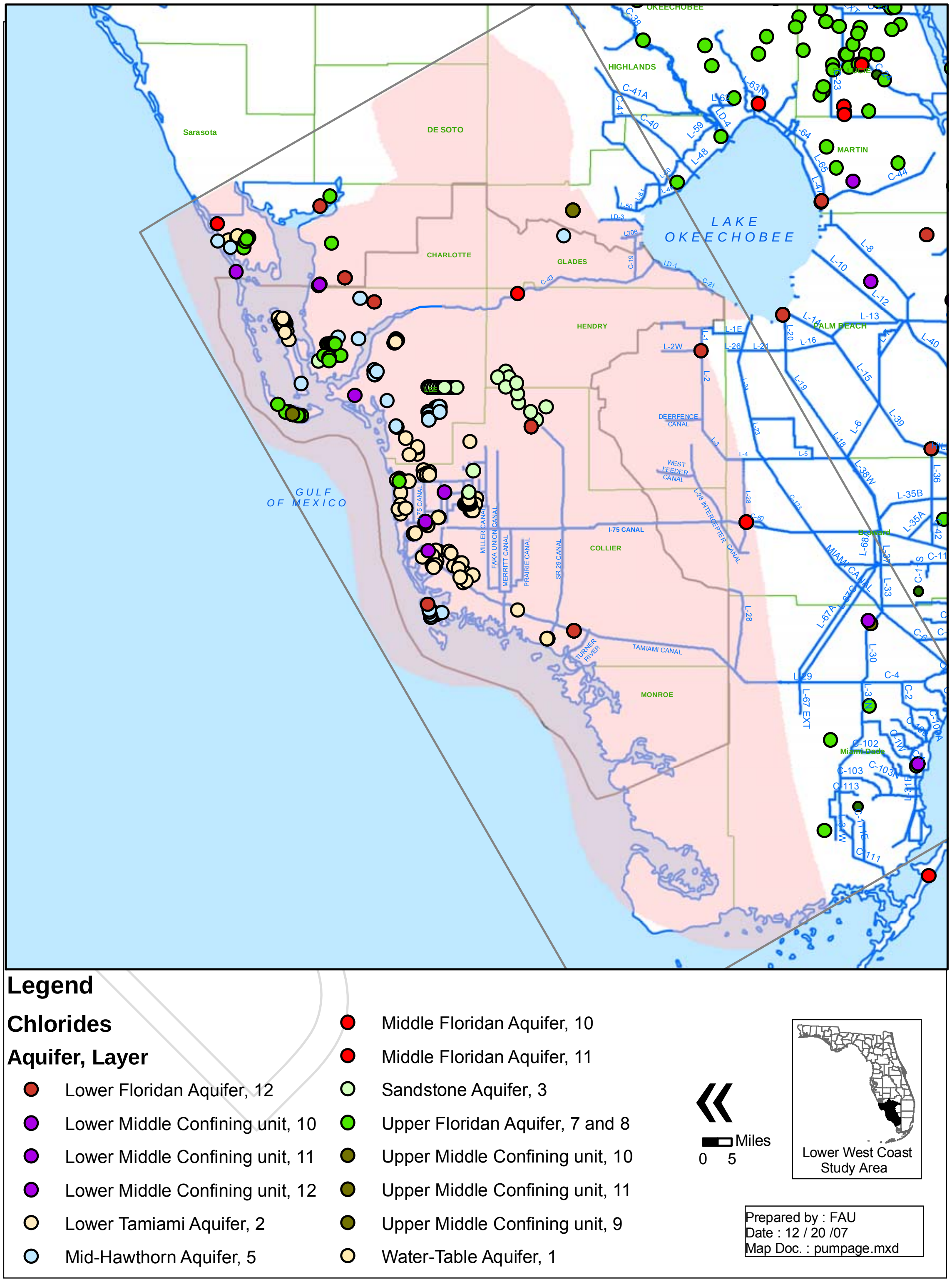

Figure 3-27. Location of monitor wells with chloride data.

Figure 3-28 through **3-32** show the regional general spatial distribution of salinity in the aquifer layers from select model layers. The salinity ranges from 0 to 35 g/L.

Due to the relatively limited development of the FAS on Florida's southeast coast, many investigators have considered current TDS concentrations as representative of pre-development conditions (Reese and Memberg 2000). Much of the LWC probably meets this condition as well, however, this is not the case with the IAS, or isolated areas of the FAS such as Marco Island or Cape Coral. Therefore, the general horizontal and vertical TDS concentration distributions in the FAS and the depth to the transition zone were used in the overall calibration process.

Individual sites in the SFWMD's database that have TDS concentration data were used for model calibration. Sites with chloride data were converted to equivalent TDS concentrations using Reese's (2000) established TDS-chloride relationships in south Florida. Several sites in the Lower East Coast Planning Area have anomalous chloride concentrations with respect to those expected at a given depth.

The range of average TDS concentrations observed in each aquifer unit in the model is summarized in **Table 3-7**. Average TDS concentrations in the IAS range in the inland areas from 60 to 1,790 ppm. The Upper Middle confining unit, Upper Floridan aquifer, and Middle Floridan aquifer are brackish but range from low (1,000 ppm) to moderately saline (10,000 to 32,000 ppm). Average TDS concentrations in the Lower Middle confining unit range from 29,500 to 33,000 ppm.

Table 3-7. Number of wells with chloride data, range of TDS concentrations and aquifer unit in the LWCFAS Model.

Aquifer Unit	Number of Wells	Minimum TDS (ppm or mg/l)	Average TDS (ppm or mg/l)	Maximum TDS (ppm or mg/l)	Model Layer(s)
water table aquifer	50	22	141	1719	1
Lower Tamiami aquifer	118	11	330	14389	2
Sandstone aquifer	47	8	61	927	3
Mid-Hawthorn aquifer	38	39	1792	8815	5
Upper Floridan aquifer	55	285	1879	10790	7-8
Upper Middle confining unit	15	1263	14020	35100	9-11
Middle Floridan aquifer	6	1520	15469	34256	10-11
Lower Middle confining unit	18	5550	29509	36682	10-12
Lower Floridan aquifer	8	19100	33226	38900	12
Total	356				

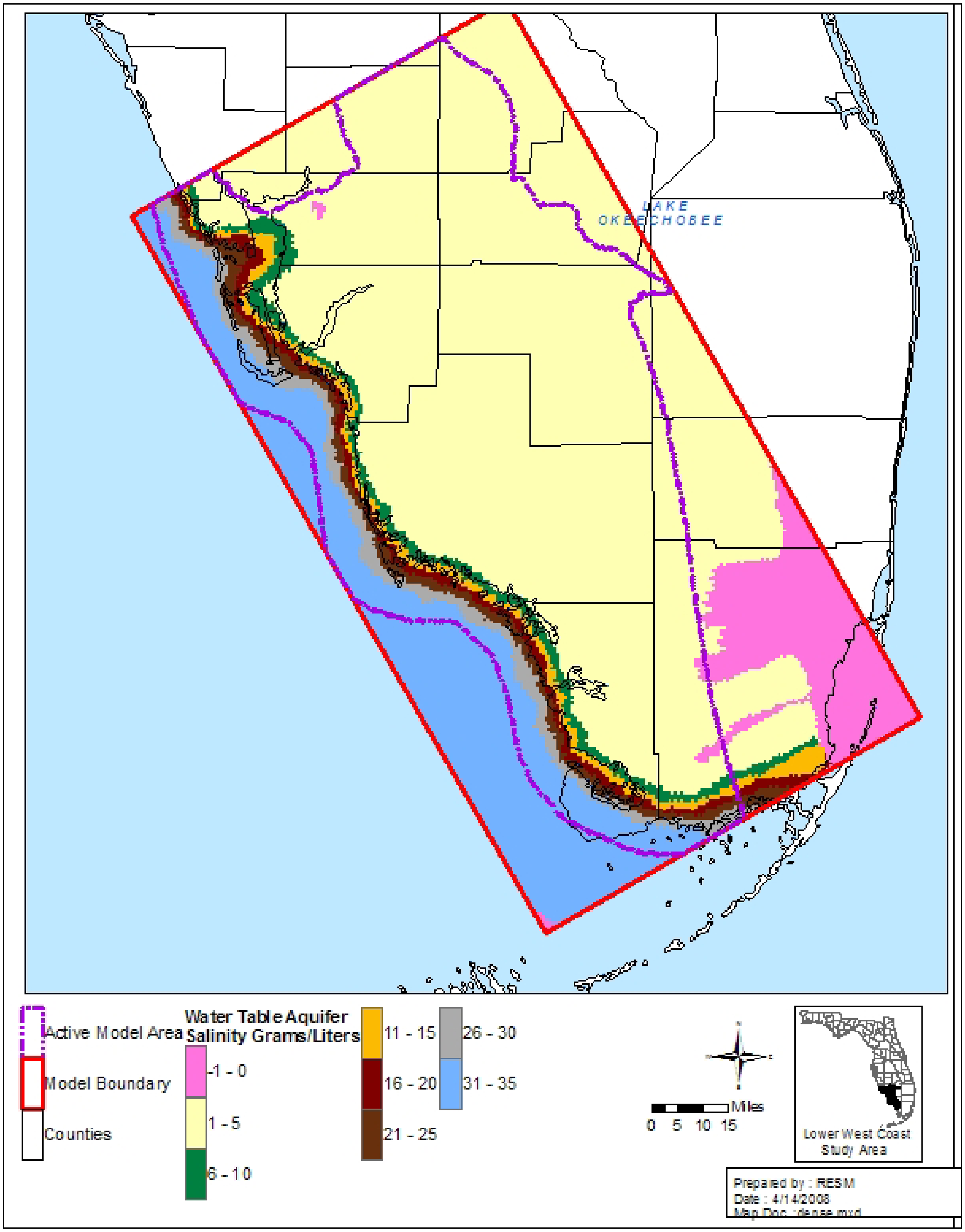

Figure 3-28. Salinity (g/L) distribution for the water table aquifer (portion of Layer 1).

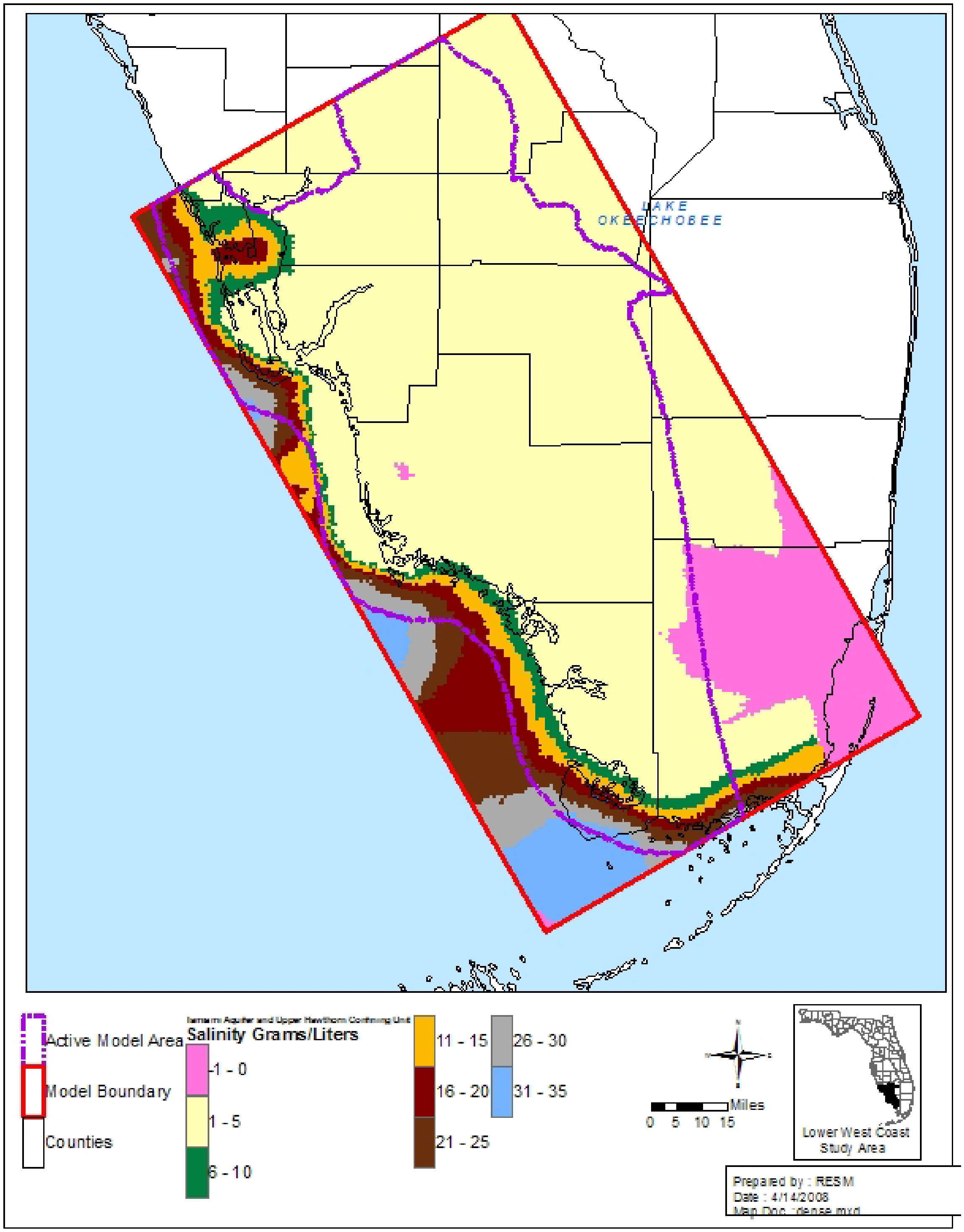

Figure 3-29. Salinity (g/L) distribution for the Tamiami aquifer and Upper Hawthorn confining unit (Layer 2).

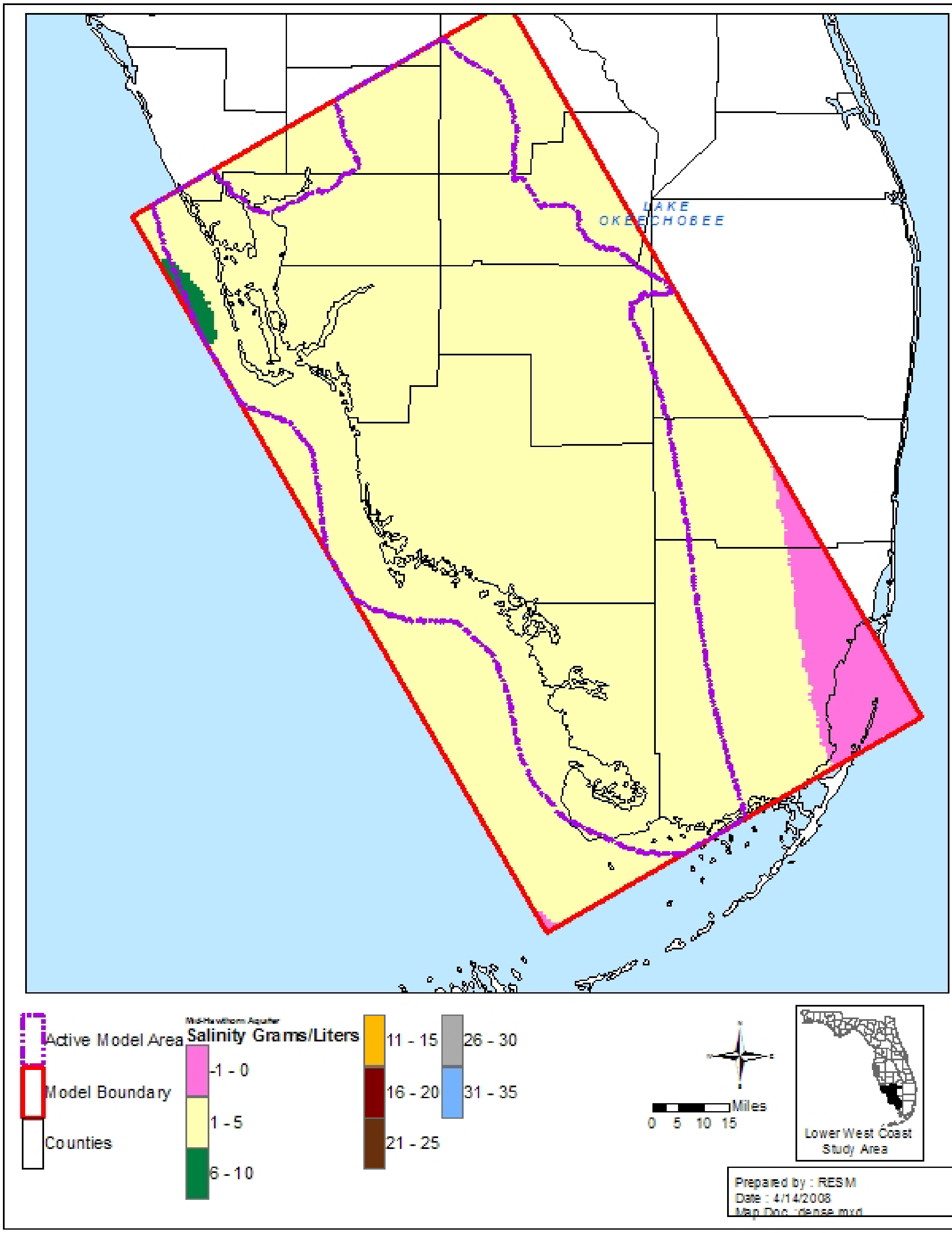

Figure 3-30. Salinity (g/L) distributions for the Mid-Hawthorn aquifer (Layer 5).

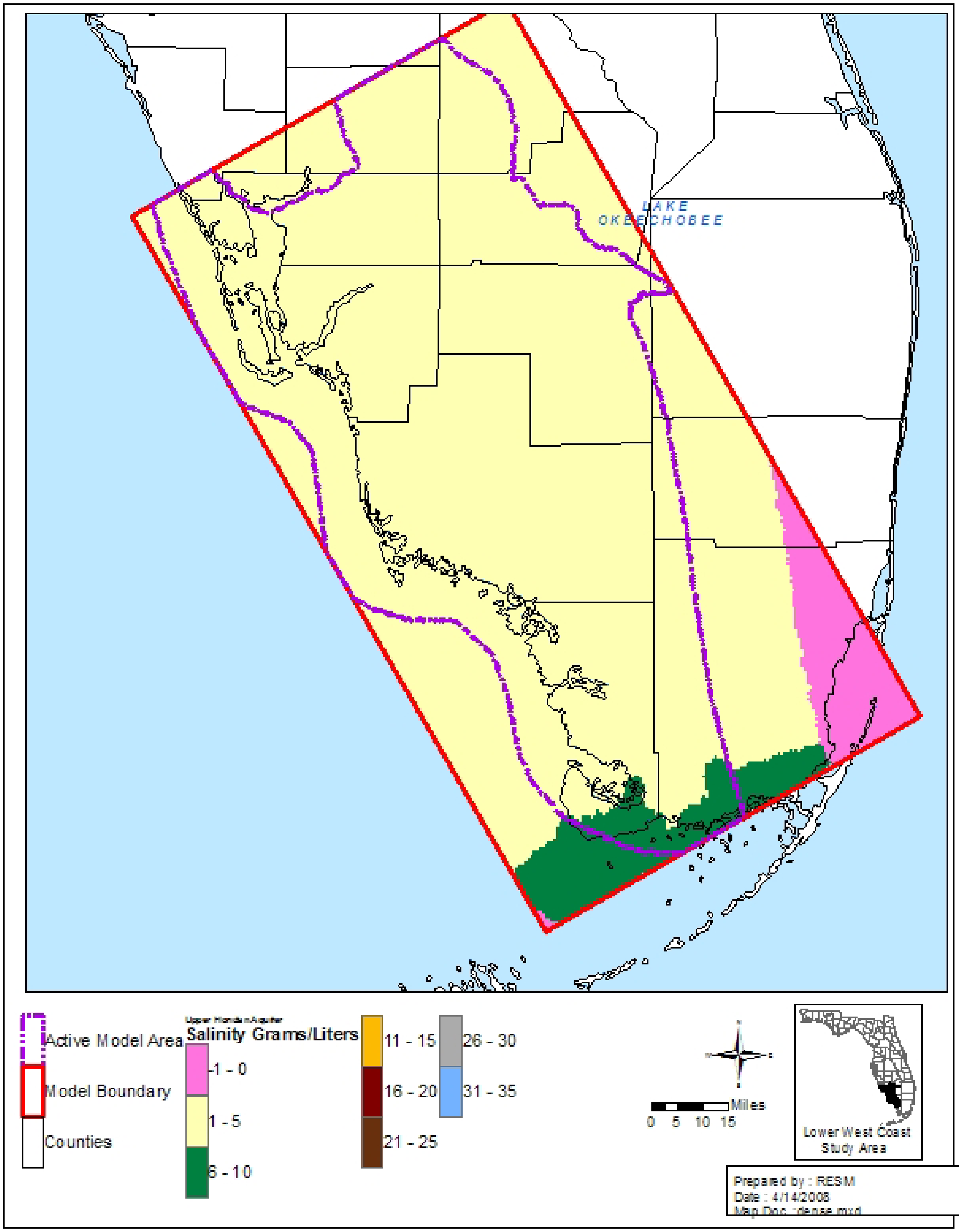

Figure 3-31. Salinity (g/L) distribution for the Upper Floridan aquifer (Layer 7).

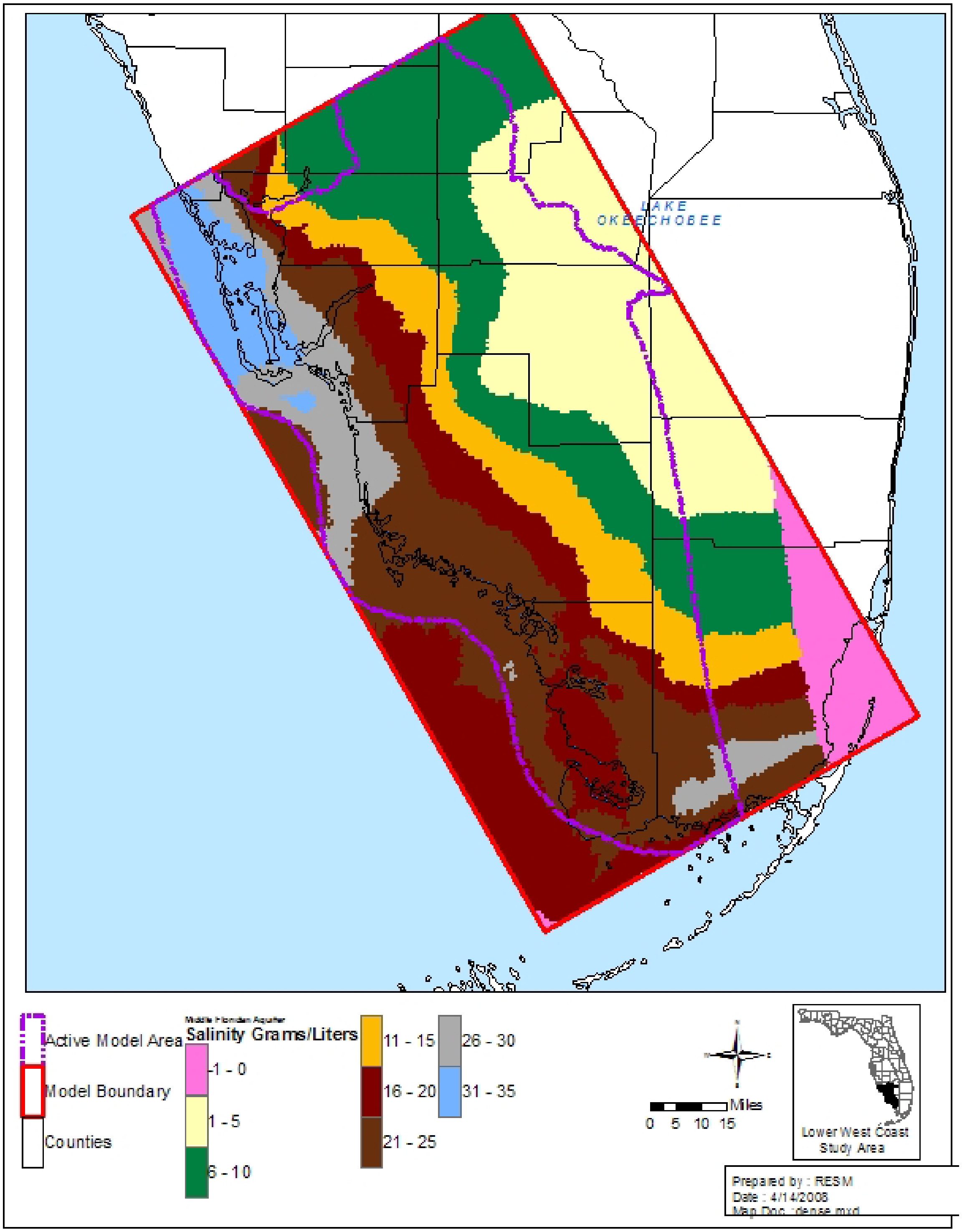

Figure 3-32. Salinity (g/L) distribution for the Middle Floridan aquifer (Layer 10).

Tidal Conditions

The tidal data were extracted from the National Oceanic and Atmospheric Administration (NOAA) Center for Operational Oceanographic Products and Service's web site by summarizing four values: Mean Lower Low Water (MLLW), Mean High Water, Mean Low Water, and Mean Higher High Water (MHHW). These values were provided for each day from 1997-2001 and were converted to daily mean tidal elevations using a FORTRAN program (Restrepo and Kuebler 2003). This program converted tidal input from a reference station with the vertical datum, MLLW (m) to an average daily value with a datum of NAVD88 (feet). Multipliers for secondary stations were provided by NOAA (2002). The shift value found by using the VERTCON (North American Vertical Datum Conversion) program developed by the National Geodetic Survey (NGS) was used to convert the values from NAVD88 (m) to NGVD29 (feet).

Two primary tidal stations were used (in Naples and Ft. Myers) along with three secondary stations (at Everglades City, Indian Key and Flamingo Bay) as shown in **Figure 3-18**. NOAA provided a set of coefficients and time delays (**Table 3-8**) that were used to generate tidal data for the secondary stations by using Naples as a reference station.

Table 3-8. Constants from the NOAA products to compute water level for the secondary stations.

Tidal Station	Time		Constant
	High Water	Low Water	
Flamingo Bay, FL	3 hr 5 min	4 hr 28 min	0.837
Indian Key, FL	47 min	1 hr 2 min	1.486
Everglades City, FL	2 hr 23 min	3 hr 25 min	0.983

Daily average values referenced to MLLW for a given secondary station were computed by multiplying the coefficient provided by NOAA for this specific station by Naples' historical data. For missing data, predicted water level data (PR) from the NOAA web site were used.

Two "imaginary" stations were created: one between Ft. Myers and Naples (Ft_Nap) and another between Indian Key and Flamingo (Ind_Fla) to avoid discrepancies that may occur due to the large distance between the two stations. This step was done by measuring the distances between the two stations and using a multiplied factor based on such a distance. The location of these stations can be seen in **Figure 3-18**.

Groundwater Withdrawals

The pumping data were obtained primarily from the SWFWMD and SFWMD. Initially, 14,392 pumping wells were identified. The data were filtered to acquire wells that were located within the study area, eliminating those that did not fall within it and also those that did not have data for the model calibration time period 1997- 2001. This elimination process reduced the total number of wells from 14,392 to 7,889. Wells were then subdivided into two broad groups: Public Water Supply (PWS) and non-PWS, **Figures 2-9** and **2-10** respectively. Non-PWS wells were further subdivided into domestic (DOM), agriculture (AGR), aquifer storage and recovery (ASR), and other (OTH), which included landscaping (LAN) and livestock (LIV). Information on pumping wells per layer/aquifer is presented in **Table 3-9**. Detailed information on wells and pumping data is presented in **Appendix D**. Locations of the wells are presented in **Chapter 2**.

Table 3-9. Pumping well data per layer/aquifer.

Layer	Aquifer Unit	Number of Wells	Well Type	Average Pumping Capacity (GPD)
2	surficial aquifer system excluding water-table	4313	AGR,IND,IRR, PWS,OTH	-597,597,246
3	Sandstone aquifer	1451	AGR,IND,IRR, PWS,OTH	-84,878,178
5	intermediate aquifer system	1512	AGR,DOM,IRR, PWS,ASR,IND,OTH	-43,243,312
7 and 8	Upper Floridan aquifer system	983	AGR,IND,IRR, PWS,ASR,OTH	-179,071,865
Total		8259		-904,790,602

Data obtained from the SFWMD included both public and non-public water supplies. Pumpage values were on a monthly basis and were measured in gallons for the non-public supply wells and millions of gallons for the public supply wells. Data from the SWFWMD were all from public water supplies and the values were on a monthly basis measured in gallons. However, to have common pumping units throughout, the non-public water supply values were converted from millions of gallons/month to gallons/month.

The total pumping capacity for each permit (the sum of the pumping capacity for each well in that permit) was distributed among the wells in the permit based on their pumping capacities (i.e., individual pumping capacity divided by total pumping capacity). The sum of the distributed ratios for the wells in the same permit must be equal to one. Then the monthly pumpage values (gallons) were converted to daily averaged pumpage values (cubic feet) to be used in the model.

Aquifer Properties

Groundwater Flow Hydraulic Properties

Hydraulic properties were compiled by the SFWMD (Richardson 2005). Data were obtained for Collier, Lee, Monroe, Charlotte and Hendry counties. No data were available for Glades County. **Appendix E** shows the hydraulic attributes for all the wells and the data collected. **Figure 3-33** shows the layout of wells with aquifer test data. The initial hydraulic properties were interpolated using the values obtained from **Figure 3-33**. The interpolation was carried out using kriging. Those values became the initial calibration parameters.

Transport Properties

In the case of deficiency of field data, it must be assumed that a set of values of porosity, longitudinal dispersivity, horizontal and vertical transverse dispersivities are uniform as possible throughout the model domain for the coupled density-dependent simulation. The selected parameters considered most representative are shown in **Table 3-10**. MT3D uses one set of values of dispersivity corresponding to one model layer.

Table 3-10. Transport parameters used in the LWCFAS Model (after Mackay et al. 1986; LeBlanc 1991; Gelhar et al. 1992).

Transport Parameters	Symbol	Common Ranges	LWCFAS Ranges
Porosity (limestones)	φ	0.01-0.22	0.18-0.22
Longitudinal Dispersivity (feet)	α_l	2-10,000	500 and 1,000
(Horizontal Transverse/Longitudinal) Dispersivity	α_t / α_l	0.01-0.10	0.10
(Vertical Transverse/Longitudinal) Dispersivity	α_v / α_l	0.010-0.0025	0.01

Longitudinal dispersivity is a function of the model area's spatial scale (Lallemand-Barres and Peaudecert, 1978; Gelhar et al 1992). Based on field experiments, it was observed that dispersivity increased with distance between source and observation point due to the large-scale heterogeneities. Averaging of any property over space will eventually arrive at a stagnation point for a given location, and so it is expected with dispersivity values. In the absence of field data "the 1/10 rule" is used, which is the longitudinal dispersivity is 1/10 of the characteristic length. The characteristic length is defined as the distance over which the maximum concentration transport is likely to occur from the entry point, at the interface between salt water and brackish water to the model boundary. In the case of the IAS and FAS, a "characteristic" length is assumed in the range of 5,000 to 10,000 feet. The corresponding range of longitudinal dispersivity is then between 600 and 6,000 feet. A value of 500 is used for Layers 1 through 6. For Layers 7 through 12, a value equal to 1,000 is used. Similarly, the transverse horizontal and vertical dispersivities are assumed using the ratios α_t / α_l equal to 0.1 and α_v / α_l equal to 0.01 in the coupled simulation.

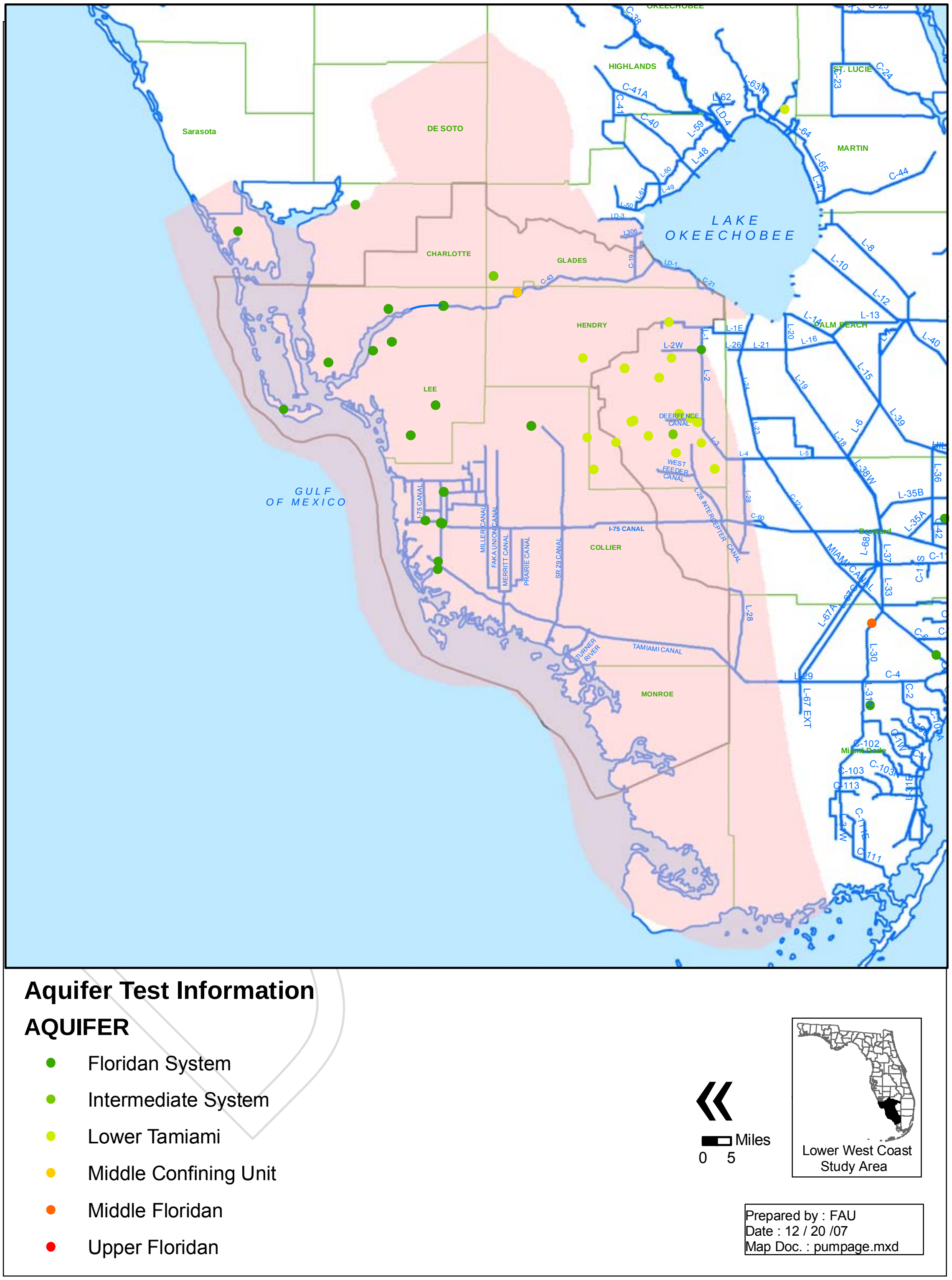

Figure 3-33. Locations of well sites with aquifer properties.

CHAPTER 4
Model Calibration

INTRODUCTION

The model calibration period for the LWCFAS Model extends from January 1, 1997 to December 31, 2001. All available field measurements over this time period were included as calibration targets. These measurements include potentiometric head and concentration data collected by the SFWMD, the USGS, and by the SWFWMD. Data used during calibration were discussed specifically in the last section of **Chapter 3**. One aspect of the modeling process was determining what observed data were available to develop the model and perform calibration. In general, the observed data should provide a sound basis for performing the water level, flow, and water quality calibration.

The goal of model calibration is to achieve the capability of simulating results that are similar to a set of field measurements within specified tolerances, produce the general groundwater flow and concentration patterns, and match temporal trends in hydraulic head and concentrations. The goal of the calibration process is to change input parameters, such as boundary conductance, horizontal and vertical conductivity, and specific storage within a predetermined range in an attempt to produce simulated heads and concentrations that match historical values.

PEST, a nonlinear, least-square, inverse modeling program developed by Doherty (2004) was used to auto-calibrate the LWCFAS Model, along with some manual calibration. The program uses Pilot Points (PPs) and Regularization parameterization scheme with SVD-Assist. This scheme is recommended for groundwater systems due to the parameter estimation process finding the "zones or regions" of higher and lower hydraulic property values; the parameter estimation process is also numerically stable (Doherty 2003). The total number of adjustable parameters (i.e., values at the PPs) depends on which decision variable (e.g., Kx and Ss) is being used. PEST estimates in this case the decision variable at all the PPs then interpolates the decision variable from the PPs to all active model cells (Doherty 2004).

PEST was applied to the model input parameters once the simulation was stable and had sound initial and boundary conditions representative of the physical system. Manual calibration was done first to prepare the model for auto-calibration and to find a quasi-steady-state condition. Although steady-state conditions rarely exist in aquifers, this groundwater modeling effort includes the quasi-steady-state analysis because the potentiometric and concentration distributions need to be more refined and more feasible in maintaining model stability while facilitating a quicker numerical solution. This prevents PEST from facing problems in the optimization procedure given an unstable groundwater model.

Many challenges arose during the initial model development: maintaining heads, avoiding dry cells, and smoothing the potentiometric and concentration fields in areas near the constant head and general head boundary conditions. After working through these challenges, transient calibration with PEST was undertaken to optimize the vertical hydraulic conductivity in the confining layers, the specific storage, and finally the horizontal hydraulic conductivity.

Most input data consisted of daily records, with the exception of wellfield withdrawals for public and non-public demands. These demands, which were mostly monthly, are the primary input stress to the model. Weekly stress periods were used for these hydrologic inputs, as well as for the general head and constant head boundary conditions (i.e., tidal and groundwater levels at the boundaries of the model). The predetermined ranges for input values were set by a combination of site-specific data (e.g., aquifer tests) or literature-cited (Freeze and Cherry 1979) values (e.g., specific storage which typically ranges from 5.0E-06 feet-1 to 1.0E-4 feet-1). The initial hydraulic parameters for the aquifers were interpolated using kriging based on results obtained from the aquifer tests presented in **Appendix E**.

For this modeling effort, transient potentiometric heads were selected as calibration targets. Targets included daily and random samples from monitoring wells with time series consisting of frequent observations (14,788 total weekly observations in 65 wells (Layers 2 through 10) over a maximum of five years. **Figure 3-26** (**Chapter 3**) shows the transient target locations and their corresponding vertical location in an aquifer.

BACKGROUND INFORMATION

As mentioned previously, the PPs and Regularization parameterization scheme with **SVD-Assist** (Doherty 2004) were used. In the PPs technique, parameter values are estimated for points lying within the model domain; then, these parameter values are spatially interpolated to the cells of the model grid using kriging. The ordinary kriging method was used; it is a stochastic estimation method that uses the information derived from the structural analysis (variogram analysis) in order to improve the estimation quality by keeping the same structure of the decision variable. When using Pilot Points and Regularization, each PP is linked to every other PP in the same zone (or linkage distance is limited by search radius). In the Regularization process, the “default system condition” prevails when there is no information to the contrary. When necessary, the Regularization deviates from the minimum amount necessary to achieve the desired level of fit. PEST's Regularization functionality will allow estimation of many parameters while ensuring that they all have reasonable values. Furthermore, it is not necessary to include unrealistic zones since PEST will find regions of spatial heterogeneity automatically, introducing said heterogeneity only where it is needed, such that model outputs match field measurements.

Using PEST's Regularization functionality may guarantee that departures from the original data are only as great as they need to be by penalizing the difference between the original data and the optimal solution. The more PPs that are used to define spatial heterogeneity, the less pronounced is the element of subjectivity in the calibration process. However, there will always be computational and numerical limits to the number of points that can be used.

In general, the more PPs that are used to characterize the distribution of a decision variable (e.g., hydraulic conductivity, storativity or conductances), the better the outcome will be for the calibration. However, during each optimization iteration, PEST requires many simulation runs, as there are adjustable parameters (sometimes twice this number). The estimation of a large number of parameters is a very computationally intensive process.

Doherty (2004) lists some advantages to calibrating with Regularized Inversion including:

- Results of parameter estimation being in synch with user's interpretation of the original data,
- Maximum statistical content being extracted from field data,
- Minimization of predictive error variances, and
- Determination of the appropriate degree of parameter parsimony through the calibration process, rather than through the user.

He also mentions the main disadvantages of calibrating with Regularized Inversion, which include:

- Importance of numerical stability. It is difficult to formulate regularization constraints that provide physically-based parameters, which provide numerical stability,
- Continued calibration not improving results. It may seem that the fit could be improved, but continued calibration may not improve the fitting due to other factors (e.g., quality of input data), and
- Very long run times, when there are many parameters (although parallel processing may help).

It is necessary to have a good deal of PPs to allow parameters to change within different zones so they can adjust to field conditions shown in model observations. However, despite such a high degree of adaptability, there is also a pressing need for faster running times. For the calibration procedure, the authors changed the time-scale from daily to weekly to help with the long run times. For instance, one calibration run with PEST called the SEAWAT-2000 executable 1,800 times. In order to use the majority of historical data (e.g., measured heads), the time-scale was not changed to bi-monthly or monthly.

Some of the advantages of calibrating with Regularized Inversion, with the addition of SVD-Assist include (also from Doherty 2004):

- The optimization estimation procedure is extremely stable (more than if only using Regularization),
- The parameter estimation process does not stop the progress of calibration prematurely because of a badly conditioned matrix,
- Calibration results with a good fit to calibration targets can be obtained with ease, and
- The original data itself are used to simplify the optimization problem.

CALIBRATION PROCEDURE

The first phase of the calibration of the LWCFAS Model focused on simulating quasi-steady-state, pre-development conditions for the establishment of reasonable boundary conditions in the Gulf of Mexico. Pre-development conditions excluded the groundwater withdrawal stresses to approximate the system behavior before the aquifers were developed for consumptive use. Selection of prescribed potentiometric heads and concentrations at the boundary (about 60,000 feet off-shore, see **Figure 3-16** for all layers of the model was critical before starting the transient calibration (i.e., second phase). The quasi-steady-state calibration for the pre-development conditions resulted in some oddities in the simulated salinity distribution (using coupled flow and transport) in areas proximal to the western boundary. There is no physical data with which to confirm or dispute the assumed model boundary.

When the coupled pre-development model was used (in the first stages), it was difficult to maintain the head in the model domain and keep several model zones stable. The coupled model also produced very unreasonable values (i.e., out of specified ranges) of concentration and hydraulic conductivities.

The coupled model's initial concentrations were interpolated from data provided by the SFWMD, with the original saltwater concentrations converted from TDS (ppm) to salinity (g/L). Based on Freeze and Cherry (1979) and as stated in the SEAWAT-2000 manual, page 18 "The value of salinity is often close to the dissolved-solids concentration. The conversion for a dilute solution is relatively simple; for example, parts per million can approximately be treated as milligrams per liter". Due to the lack of data, some dummy values of salinity were used along the coast (32,500 ppm) for the top layers (1 through 3) while setting up the initial conditions for the coupled model. The dummy values helped bound the interpolated values.

This quasi-steady-state simulation helped to refine both the boundary conditions and concentrations until the surface around the boundary was smooth. Then, the constant head and the general head boundaries could be set for the transient model. The model simulation length consisted of one stress-period with 10,000 time-steps. This set up was long enough to produce a “steady-state” solution at the boundaries. To find the western boundary heads for Layers 4 through 11, the model was executed leaving the original constant head cells active until said cells reached equilibrium (at about 10,000 days). Then, the model-generated values (from the previous run) were input back into the model to refine the constant head boundary cells. The rationale behind this approach is that the actual boundary conditions extend far beyond the limits of the conceptualized model, and that those actual boundaries are unknown. Maps of initial starting heads are presented in **Appendix K**, Figures K-1 through K-10, representing Layers 2 through 11, respectively.

For the LWCFAS Model transient calibration, in order to have reasonable running times, the original 3,000 feet by 3,000 feet model was aggregated into a coarser model with a resolution of 12,000 feet by 12,000 feet; this model was run uncoupled and has 12 layers, 72 rows, 37 columns and 260 weekly stress periods. The use of the uncoupled model is justifiable, as elaborated in **Chapter 3**. In the decision process for the calibration, computer time for a simulation was also taken into consideration. A typical simulation (using the 12,000 feet by 12,000 feet cell uncoupled model) requires approximately 156 seconds (0.04 hours) of CPU. The 3,000 feet by 3,000 feet cell uncoupled model requires approximately 4,700 seconds (1.3 hours) of CPU. The simulation was also run for both of the aforementioned models using a coupled version; in this case, approximately 4,800 seconds (1.34 hours) of CPU was needed for the former and 134,000 seconds (37 hours) for the latter. All cases use a 3.2 GHz Intel Xeon processor with 4 MB RAM.

For the transient, uncoupled calibration, a sequential calibration approach (with three steps) was used. The first step estimated the decision variables at PPs at a coarser resolution. The algorithm based upon sequential optimization steps increased the number of PPs to produce spatial disaggregation of the domain. However, initial conditions and the assumption of the “convexity” function should be used in order to make a good tool, which increases the chances of obtaining better results at each step. This procedure was followed since a large model is being calibrated and PEST is a very calculation intensive program. In this approach, the same type of objective function was used. Notice that a strong weighting (8 or 10) on the deeper layers (5 through 11) was used to provide better estimates of the lower-zone parameters, because those layers are the focus of the modeling effort. However, the procedure took into account the information of the upper layers with a minimum weight.

For each stage of the calibration process, a series of independent single-calibration runs were performed for three decision variables. Transient calibration was undertaken to determine sequentially: vertical hydraulic conductivity in the confining layers, then the specific storage of aquifer systems, and finally the horizontal hydraulic conductivity. An attempt was made to calibrate the three decisions simultaneously.

However, the size of the problem overshadows the current computer speeds and also calculation capabilities.

Step 1. The initial conditions created by the quasi-steady-state simulation were used to start the transient calibration. The PPs were located every 8 cells, or the equivalent of every 96,000 feet in the x and y directions. The total number of PPs was 27 per layer. The total number of PPs in a model simulation depends on the decision variables (from 162 to 324 PPs). The range of values for horizontal hydraulic conductivity was purposefully constrained, trying to remain true to the actual aquifer test data. The range in Kx was considered the best data available to this model. The optimal solution for the three decision variables was found using PEST. Several rounds of Step 1 were carried out until the solution did not change substantially. One time, the conductance of the general head was changed manually to reduce the flow to the boundary.

Step 2. The second step in this approach builds on Step 1 by increasing the number of PPs. The PPs were located every 7 cells, or the equivalent of every 84,000 feet in the x and y directions. The total number of PPs was 36 per layer. The total number of PPs in the model simulation was from 210 to 420. The parameter space for the horizontal hydraulic conductivity was kept very tight as described in Step 1. The optimal solution for the three decision variables was found, again, at this stage. One round of Step 2 was carried out. The solution did not change substantially for Kx.

Step 3. After completion of the second step, an additional round of runs was made to allow for refinement of the lower-layer parameters starting with the solution in Step 2. The PPs are located every 6 cells, or the equivalent of every 72,000 feet in the x and y directions (about 49 PPs per parameter per layer). The total number of PPs in this simulation was from 294 to 490. The solution did not change substantially for specific storage (Ss) and Kx.

In each step, the following procedure was followed. For the vertical hydraulic conductivity, the PPs were used in Layers 1, 2, 4, 6, 9 and 11. In Layer 1, the original Kz was used as a starting point, with an upper limit defined as one order of magnitude of the starting value and three orders of magnitude (0.001) for a lower limit. The limits for the other confining layers were set from 1.0E-9 to 2.E+1 and the initial values were based on the few published leakance values available. In addition, several geological fractures are expected in the model domain. The PPs used for the second parameter optimized (Ss), and were located in all the aquifers systems (i.e., Layers 2, 3, 5, 7, 8, and 10). A calibration for the Ss for the confining units demonstrated that Ss did not play any major role in influencing the model results. After running the optimization, the objective function did not improve. The final calibrated parameter was the horizontal hydraulic conductivity in all the aquifer systems (i.e., Layers 2, 3, 5, 7, 8, and 10).

This procedure combines the strengths of the manual and automatic calibration strategies. The result is a multistep automatic calibration scheme that follows a progression of steps that end up providing a better calibration with acceptable parameter estimates.

For the PEST calibration of the vertical hydraulic conductivity, Kz, the number of superparameters was set between 12 and 20 percent of the total number of parameters. For example, the total number of parameters for this Kz calibration in Step 3 was 291, equivalent to 40 superparameters.

The upper and lower bounds of the horizontal conductivity were set to 35 percent above and below the original data provided by the SFWMD. The final results for the horizontal conductivities are relatively close to the field-measured data for this parameter. The advantage of this procedure is that we are changing the least known parameter so that changes in the horizontal conductivity in the aquifer units remain physically meaningful. The image in **Figure 4-1** shows the Pilot Point distribution for Step 3. **Appendix L** provides the optimized horizontal hydraulic conductivity maps.

This entire process was accomplished through a combination of GWVistas utilities and some changes in the PEST batch file that run several PEST utility programs, as well as the updated SEAWAT 2000.

The process of assigning weights to observations is discussed in USGS report 98-4005 (Methods and Guidelines for Effective Model Calibration) as well as the PEST manual. The USGS report provides a statistical basis to reflect measurement errors and the PEST manual discusses assigning weights that include different types of observations in the model calibration. The weights discussed in these reports may only be applied to locations where the observations were collected. In the current optimization procedure, two weights for the observations were used. For information on Layers 1 through 4, weights equal to one are set equal to 1. For Layers 5 through 11, weights were set equal to 8. These criteria put more weight to the focus area of this project – Layers 5 through 12.

It is worth mentioning that one of the advantages of this optimization technique is the use of "prior information", so that by default, the calibration parameters have the original value assigned by the SFWMD and don't change unless there is a clear benefit in the model calibration, especially since there is a "penalty" for wandering away from the original values.

Appendix H shows the observed versus modeled potentiometric head levels and the statistics for each of the observation wells in the aggregated model with a resolution of 12,000 feet by 12,000 feet. **Appendix I** shows the same head level comparison, albeit with a resolution of 3,000 feet by 3,000 feet. For Layers 2 through 4, an interval of +/- 3 feet is used to define the interval around the historical value. For Layers 5 through 10, an interval of +/-5 is used.

It is important to mention that the calibration procedure was repeated for the vertical conductivity using a 6,000 feet by 6,000 feet model grid. This time, up to 10 additional PPs were added around the available monitor wells for the layers in the Floridan aquifer system. The previously calibrated vertical conductivity was used as a starting point. For this new, more refined calibration round, there were no appreciable changes in the objective function (root mean squared error). The authors think this may be due to a lack of data (for monitor wells) in the Floridan aquifer system and that kriging could create very good interpolation results for the parameters.

Nevertheless, the model can be run as a coupled model, and once new data becomes available, it can be integrated into the project and new density-dependent simulations can be run. A simulation span of no greater than 20 years time can be used without making any significant calibration changes to the concentrations.

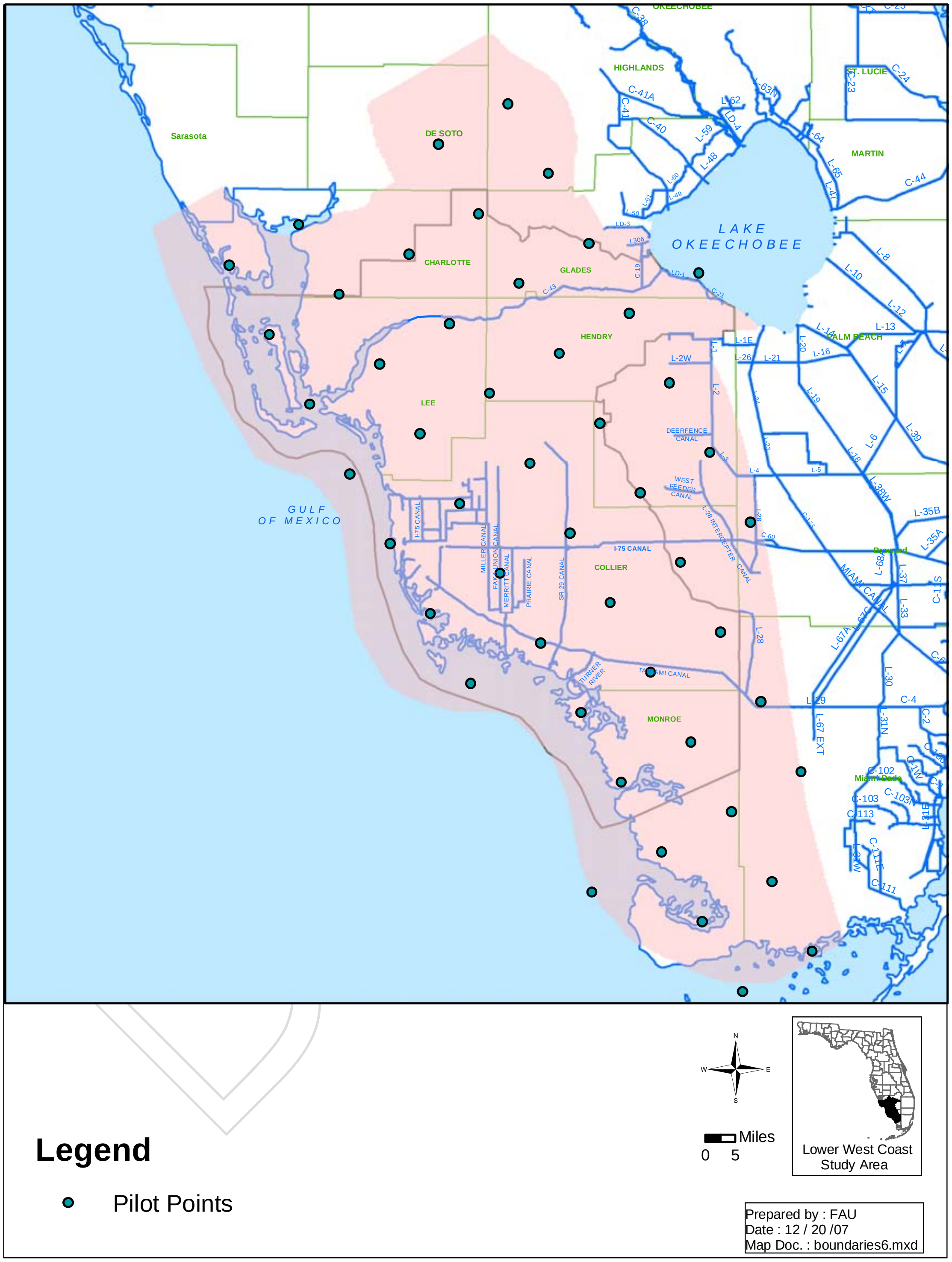

Figure 4-1. Pilot Point distribution (every seven cells) for all optimized layers.

CALIBRATION STATISTICS

The auto-calibration software PEST performs the function of minimizing the errors in the objective function while considering the constraints. However, model results have been summarized using three statistics: mean absolute error, root mean square error, and percentage of time that simulated head lies within a plus or 3 feet in Layers 1 through 4 and 5 feet in Layers 5 through 10 of the observed heads.

The mean absolute error (MAE) is the mean of the absolute value of the differences between measured and simulated heads. The root mean square (RMS) error, or the standard deviation, is the average of the squared differences in measured and simulated heads.

These statistics were used to set calibration criteria for model Layers 2 through 10. Layers 2 through 4 are considered calibrated when the simulated heads fall within 3 feet of the measured heads 60 percent of the time. Layers 5 through 10 are considered calibrated when the simulated heads fall within 5 feet of the measured heads 60 percent of the time. Different criteria were used for the model layers due to the lack of information and the complexity of the model.

CALIBRATION RESULTS

Tables 4-1 and **4-2** show the resulting statistics for the two, uncoupled models. The aggregated calibrated model is a 12,000 feet by 12,000 feet model, and the disaggregated one model has a resolution of 3,000 feet by 3,000 feet. Note that the calibration targets are not evenly distributed. There are more observations in the upper model layers than in the deeper model layers. The calibration statistics meet the designated calibration criteria 80 percent and 72 percent of the time, respectively.

Table 4-1. Statistics for the 12,000 feet by 12,000 feet uncoupled model.

STATION	Layer	MAE	RMS	+/-3/5 feet band (% of time)
11-00017-W_C490	2	1.07	0.98	91
11-00017-W_C491	2	1.30	0.85	96
11-00017-W_C528	2	1.14	0.83	98
11-00044-W_LRCMW-1	2	1.08	0.81	96
11-00044-W_LRCMW-2	2	0.63	0.56	100
11-00076-W_SLSF-MW1	2	1.88	0.98	90
11-00076-W_SLSF-MW2	2	1.73	0.74	97
11-00076-W_SLSF-SW1	2	0.72	0.51	100

STATION	Layer	MAE	RMS	+/-3/5 feet band (% of time)
11-00179-W_ECOM237	2	0.14	0.29	100
11-00179-W_ECOM597	2	0.36	0.26	100
11-00179-W_ECOM598	2	0.60	0.26	100
11-00179-W_ECOM599	2	0.81	0.59	100
11-00628-W_2	2	2.37	0.99	76
3AS3W1	2	0.44	0.11	100
3AS3W2	2	0.38	0.12	100
3AS3W3	2	0.34	0.13	100
3AS3W4	2	0.37	0.12	100
C-1004R	2	3.16	2.04	49
C-1063	2	2.17	0.97	79
C-1065	2	0.32	0.18	100
C-1071	2	1.65	1.59	81
C-1083	2	3.63	1.87	40
C-492	2	2.29	1.55	52
C-496	2	1.57	0.77	99
C-690	2	0.82	0.40	100
CRS04FM	2	2.57	0.44	85
CRS05NM	2	0.22	0.10	100
CRS06FM	2	2.36	0.50	95
CRS06NM	2	2.48	0.47	91
G-620_B	2	0.52	0.32	100
CRS01NM	2	1.29	0.26	100
CRS02FM	2	3.27	0.75	37
CRS02NM	2	3.98	0.29	1
11-00628-W_1	3	4.65	1.92	20
11-00628-W_3	3	3.38	1.25	33
C-1072	3	1.52	1.32	86
C-688	3	2.16	1.33	68
C-951	3	2.26	1.02	74
C-988	3	2.47	1.26	63

STATION	Layer	MAE	RMS	+/-3/5 feet band (% of time)
L-1994	3	3.16	2.52	60
L-2194	3	2.39	1.68	69
L-2550	3	3.92	7.43	64
L-5747	3	3.29	2.09	50
L-727	3	0.98	0.94	93
L-729	3	3.19	2.72	60
CRS01FM	3	1.41	0.60	100
HE-517	3	5.77	1.70	4
HE-556	3	3.96	3.73	56
C-1079	5	4.01	2.70	74
CH-11333	5	1.19	0.83	100
CH-12882	5	2.21	1.66	93
L-1993	5	3.20	1.81	83
L-2193	5	4.19	3.50	65
CH-11334	7	2.22	1.82	89
I75-TW-MZ1	7	0.51	0.42	100
I75-TW-MZ2	7	0.69	0.47	100
HL-12955	8	1.97	1.47	97
LAB-TW-MZ1	8	0.98	0.60	100
DS-10933	10	2.06	1.52	96
DS-17816	10	2.83	1.90	90
HL-13239	10	2.20	1.65	90
IWSD-TW-MZ2	10	22.45	0.65	0
IWSD-TW-MZ3	10	2.86	1.34	98
LAB-TW-MZ3	10	7.19	1.06	1

Table 4-2. Statistics for the 3,000 feet by 3,000 feet uncoupled model.

STATION	Layer	MAE	RMS	+/-3/5 ft band (% of time)
11-00017-W_C490	2	3.64	1.53	36
11-00017-W_C491	2	1.14	0.80	98
11-00017-W_C528	2	0.71	0.45	100
11-00044-W_LRCMW-1	2	1.36	0.91	92
11-00044-W_LRCMW-2	2	0.74	0.48	100
11-00076-W_SLSF-MW1	2	2.03	1.01	85
11-00076-W_SLSF-MW2	2	1.83	0.71	94
11-00076-W_SLSF-SW1	2	0.74	0.51	100
11-00179-W_ECOM237	2	0.14	0.28	100
11-00179-W_ECOM597	2	0.28	0.34	100
11-00179-W_ECOM598	2	0.49	0.32	100
11-00179-W_ECOM599	2	0.65	0.60	100
11-00628-W_2	2	2.21	1.06	75
3AS3W1	2	0.23	0.07	100
3AS3W2	2	0.20	0.05	100
3AS3W3	2	0.15	0.08	100
3AS3W4	2	0.20	0.06	100
C-1004R	2	2.68	1.81	56
C-1063	2	1.99	0.89	87
C-1065	2	0.29	0.23	100
C-1071	2	1.64	1.58	81
C-1083	2	2.32	1.54	66
C-492	2	2.25	1.62	53
C-496	2	2.14	0.90	87
C-690	2	0.69	0.45	100
CRS04FM	2	2.57	0.44	85
CRS05NM	2	0.19	0.10	100
CRS06FM	2	1.29	0.50	100
CRS06NM	2	1.39	0.49	100
G-620_B	2	0.79	0.28	100

STATION	Layer	MAE	RMS	+/-3/5 ft band (% of time)
CRS01NM	2	1.29	0.26	100
CRS02FM	2	2.83	0.75	50
CRS02NM	2	3.54	0.31	5
11-00628-W_1	3	3.20	1.48	41
11-00628-W_3	3	3.42	1.25	33
C-1072	3	1.50	1.29	86
C-688	3	2.43	1.34	63
C-951	3	1.32	0.83	97
C-988	3	1.69	1.20	86
L-1994	3	3.36	2.78	57
L-2194	3	2.47	1.76	67
L-2550	3	3.66	6.42	66
L-5747	3	3.70	2.24	41
L-727	3	1.01	0.72	99
L-729	3	3.15	2.53	61
CRS01FM	3	1.40	0.60	100
HE-517	3	5.92	1.71	3
HE-556	3	4.50	2.90	33
C-1079	5	3.74	2.94	78
CH-11333	5	5.85	1.36	27
CH-12882	5	2.16	2.02	89
L-1993	5	3.74	2.99	65
L-2193	5	5.12	3.89	58
CH-11334	7	12.97	2.12	0
I75-TW-MZ1	7	6.14	0.84	3
I75-TW-MZ2	7	5.82	0.92	12
HL-12955	8	3.72	2.08	73
LAB-TW-MZ1	8	0.98	0.58	100
DS-10933	10	3.56	2.38	72
DS-17816	10	3.56	2.93	74
HL-13239	10	2.20	1.47	96

STATION	Layer	MAE	RMS	+/-3/5 ft band (% of time)
IWSD-TW-MZ2	10	20.41	0.66	0
IWSD-TW-MZ3	10	1.74	1.09	100
LAB-TW-MZ3	10	7.21	1.08	1

Calibration scatter plots show calculated vs. observed values of heads in a model. Three plots (12,000 feet by 12,000 feet coupled and uncoupled; and 3,000 feet by 3,000 feet uncoupled) are used to analyze calibration targets within the model domain, specifying groups of observations per aquifer system. The plots are depicted in **Figures 4-2** through **4-6**, corresponding to each model variation. These plots are useful for interpreting the LWCFAS Model because the plots show the difference in resolution and solution method (uncoupled versus coupled). Calibration statistics are displayed on the scatter plot.

Figure 4-2 is a plot of the observed versus simulated data for Layers 2, 3, 5, 7, and 10 for the 12,000 feet by 12,000 feet uncoupled model. Most points are clustered in a cloud. The cloud is close to an imaginary line with a slope of 1:1 (historical/observed). However, there are some outliers. **Table 4-3** provides the standard error and correlation coefficient (r-value) for each layer. The r-values and graph indicate that there is a good linear relationship between the observed and simulated data for all layers.

Figures 4-3 through **4-4** are scatter plots for the 3,000 feet by 3,000 feet uncoupled and the 12,000 feet by 12,000 feet coupled models, respectively. The results are similar to **Figure 4-2**. **Tables 4-4** and **4-5** provide the standard error and correlation coefficient for the 3,000 feet by 3,000 feet uncoupled and 12,000 feet by 12,000 feet coupled models, respectively.

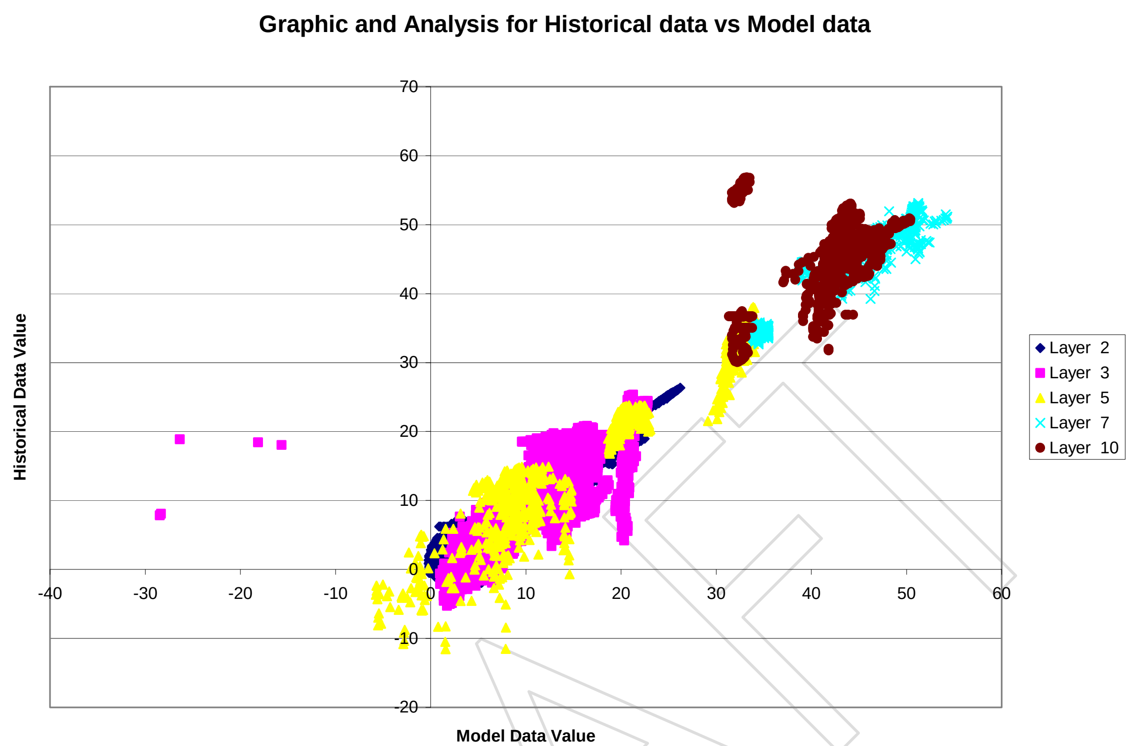

Figure 4-2. Calibration scatter plots showing calculated vs. observed head values for the 12,000 feet by 12,000 feet uncoupled model.

Table 4-3. Standard error and correlation coefficient for 12,000 feet by 12,000 feet uncoupled model.

Layer	Standard Error (ft)	Correlation Coefficient
2	1.97	0.95
3	4.12	0.75
5	3.50	0.95
7	1.68	0.97
10	6.99	0.40

Model statistics indicate that the model does an acceptable job of matching the historical data between 1997 and 2001. The combination of reasonable parameter distributions and a good fit between modeled values and field observations indicates that the model can be useful for evaluating regional groundwater issues where the concentration is not expected to change significantly over long periods of time.

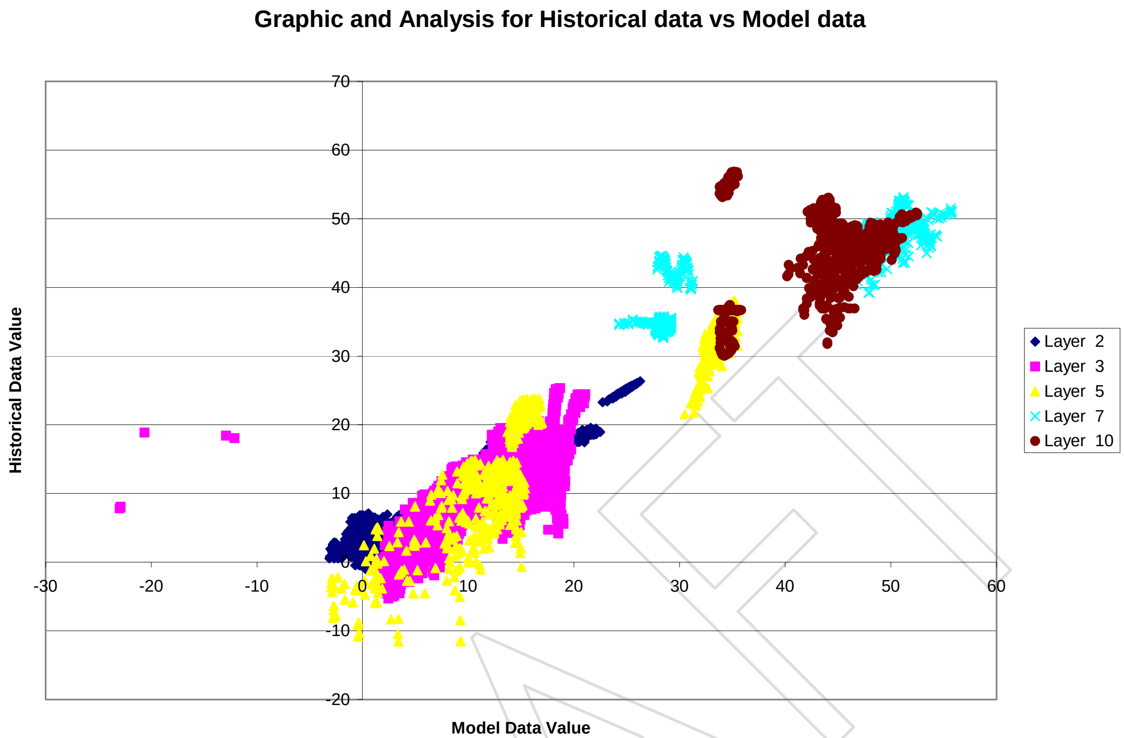

Figure 4-3. Calibration scatter plots show calculated vs. observed values of heads in the 3,000 feet by 3,000 feet uncoupled model (to be updated).

Table 4-4. Standard error and correlation coefficient for the 3,000 feet by 3,000 feet uncoupled model.

Layer	Standard Error (ft)	Correlation Coefficient
2	1.94	0.96
3	3.99	0.76
5	4.97	0.91
7	5.34	0.91
10	7.40	0.32

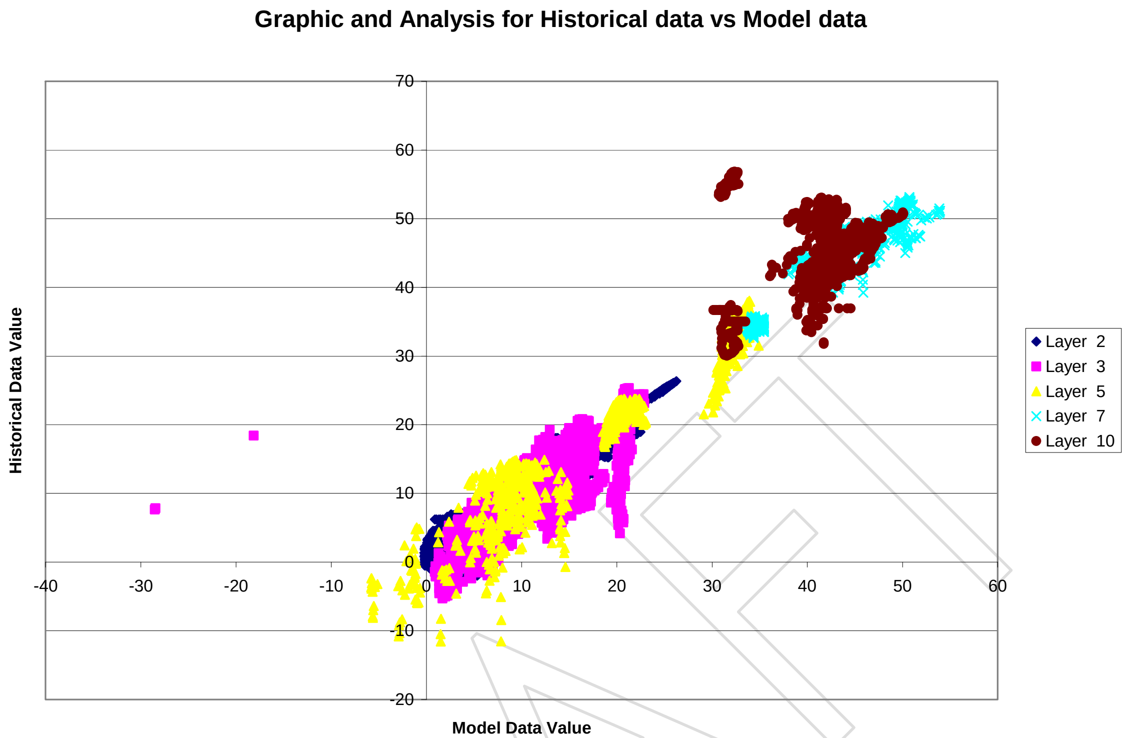

Figure 4-4. Calibration scatter plots show calculated vs. observed values of heads in the 12,000 feet by 12,000 feet coupled model.

Table 4-5. Standard error and correlation coefficients for the 12,000 feet by 12,000 feet coupled model.

Layer	Standard Error (ft)	Correlation Coefficient
2	1.96	0.95
3	3.73	0.79
5	3.48	0.95
7	1.69	0.96
10	7.34	0.32

VOLUMETRIC BUDGET

Table 4-6 presents the volumetric budget for the 12,000 by 12,000 uncoupled model. Constant head flows represent the largest inflows and outflows (50% and 57% respectively). Storage is the second largest inflow (34%); but the third largest outflow (12%). Head dependent boundaries are the third largest inflows (17%); but second largest outflows (24%).

Well inflows are relatively small (0%) but wells represent 7 percent of the outflow. The well inflows are ASR and injection wells.

The DCDT values are the changes in fluid volume due to change in concentration (Guo and Langevin 2002).

Table 4-6. Volumetric flows for the 12,000 feet by 12,000 feet uncoupled model.

INFLOW	VOLUME (ft^3)	PEERCENTAGE
STORAGE	6.86E+13	34%
CONSTANT HEAD	1.01E+14	50%
WELLS	2.4E+10	0%
HEAD DEP BOUNDS	3.38E+13	17%
DCDT	0.00E+00	0%
TOTAL IN	2.03E+14	100%
OUTFLOW	**VOLUME (ft^3)**	**PERCENTAGE**
STORAGE	2.48E+13	12%
CONSTANT HEAD	1.17E+14	57%
WELLS	1.37E+13	7%
HEAD DEP BOUNDS	4.82E+13	24%
DCDT	0.00E+00	0%
TOTAL OUT	2.03E+14	100%

Table 4-7 provides the volumetric flows for the 3,000 feet by 3,000 feet uncoupled model. Similar to the 12,000 feet by 12,000 feet model, constant heads represent the largest inflows and outflows (62% and 50%, respectively). However, storage is the second largest inflow (22%) and outflow (27%).

Table 4-7. Volumetric flows for the 3,000 feet by 3,000 feet uncoupled model.

INFLOW	Volume(ft^3)	Percent
STORAGE	5.12E+13	22%
CONSTANT HEAD	1.43E+14	62%
WELLS	2.40E+10	0%
HEAD DEP BOUNDS	3.70E+13	16%
DCDT	0	0%
TOTAL IN	2.32E+14	100%
OUTFLOWS	**Volume(ft^3)**	**Percent**
STORAGE	6.20E+13	27%
CONSTANT HEAD	1.16E+14	50%
WELLS	1.37E+13	6%
HEAD DEP BOUNDS	4.00E+13	17%
DCDT	0	0%
TOTAL OUT	2.32E+14	100%

Tables 4-8 presents the results for the 12,000 feet by 12,000 feet coupled model. The cumulative volume is slightly larger. With the coupled version, there are some small flows from the changes in concentration (DCDT). However, percentages are fairly close to the uncoupled version (**Table 4-6**).

Table 4-8. Volumetric budget for the 12,000 feet by 12,000 feet coupled model.

INFLOW	VOLUME (ft^3)	PERCENTAGE
STORAGE	7.49E+13	35%
CONSTANT HEAD	1.04E+14	49%
WELLS	2.43E+10	0%
HEAD DEP BOUNDS	3.39E+13	16%
DCDT	7.84E+11	0%
TOTAL IN	2.13E+14	100%
OUTFLOW	**VOLUME (ft^3)**	**PERCENTAGE**
STORAGE	2.61E+13	12%
CONSTANT HEAD	1.25E+14	58%
WELLS	1.37E+13	6%
HEAD DEP BOUNDS	4.70E+13	22%
DCDT	1.80E+12	1%
TOTAL OUT	2.13E+14	100%

SENSITIVITY ANALYSIS

After calibrating the LWCFAS Model, a sensitivity analysis was performed to quantify how variations in selected model parameters affect the calibrated model. A sensitivity analysis is defined as "a quantitative evaluation of the impact of variability or uncertainty in model inputs on the degree of calibration of a model and on its results or conclusions" (ASTM 2002). Sensitivity runs are usually conducted to test the magnitude of the model's response on the range of simulated outputs (i.e., simulated heads) to changes in aquifer parameters, stresses, and boundary conditions.

Parameters and Methodology

When performing sensitivity analysis for LWCFAS Model, the selected input parameters vary within an acceptable range, which were based on the range of data for each parameter used to develop and calibrate the model, and also chosen to ensure that the sensitivity runs converge. During the sensitivity analysis, one parameter was changed at a time so the effect of its variations on the model could be individually assessed.

The LWCFAS Model was calibrated for two modes (uncoupled and coupled) with two different grid sizes (3,000 feet by 3,000 feet and 12,000 feet by 12,000 feet) accordingly. The model system includes several aquifers (UFA, MFA, etc.) and confining units (aquitards) with flow between aquifers controlled by vertical permeability of confining units. In aquifers, flow is generally affected by aquifer characteristics (i.e., hydraulic conductivity and specific storage) under certain hydrologic gradients and stresses. In the coupled models, solute transport modeling is coupled with flow modeling, simulating the spatiotemporal changes in solute concentrations, densities and thus heads. Dispersivity that varies over several orders of magnitude may largely affect solute transport in aquifers since dispersion coefficients are large due to relatively high Darcian velocities.

Table 4-9 shows sensitivity analysis parameters and their multipliers. The tested parameters mainly included vertical hydraulic conductivity (Kz) of confining units (Layers 2, 4, 6, 9, and 11), horizontal hydraulic conductivity (Kx), specific storage (Ss), and longitudinal dispersivities (v) in the primary aquifers (Layers 3, 5, 7, 8 and 10). In addition to changes in specific confining units and aquifers, global changes of Kz, Kx and Ss in all layers are also included. For each parameter, several model runs were completed using the different multipliers (**Table 4-9**). The simulation period for the sensitivity analysis, January 1, 1997 to December 31, 2001, was the same as the calibration period of the model.

Table 4-9. Parameters and multipliers of Sensitivity Analysis for the LWCFAS Model.

Parameters	Multipliers					
Vertical Hydraulic Conductivity Kz (Layer 2, Tamiami aquifer, and Upper Hawthorn confining unit)	0.1	0.5	2	10		
Vertical Hydraulic Conductivity Kz (Layer 4, Mid-Hawthorn confining unit)	0.1	0.5	2	10		
Vertical Hydraulic Conductivity Kz (Layer 6, Lower Hawthorn confining unit)	0.1	0.5	2	10		
Vertical Hydraulic Conductivity Kz (Layer 9, Upper Middle confining unit)	0.1	0.5	2	10		
Vertical Hydraulic Conductivity Kz (Layer 11, Lower Middle confining unit)	0.1	0.5	2	10		
Vertical Hydraulic Conductivity Kz (All layers)	0.5	0.7	0.95	1.05	2	5
Horizontal Hydraulic Conductivity Kx (Layer 3, Sandstone aquifer)	0.1	0.5	2	10		
Horizontal Hydraulic Conductivity Kx (Layer 5, Mid-Hawthorn aquifer)	0.1	0.5	2	10		
Horizontal Hydraulic Conductivity Kx (Layers 7 and 8, UFA)	0.1	0.5	2	10		
Horizontal Hydraulic Conductivity Kx (Layer 10, MFA)	0.1	0.5	2	10		
Horizontal Hydraulic Conductivity Kx (All layers)	0.5	0.7	0.95	1.05	2	5
Specific Storage Ss (Layers 7 and 8, UFA)	0.01	0.1	10	100		
Specific Storage Ss (Layer 10, MFA)	0.01	0.1	10	100		
Specific Storage Ss (All layers)	0.01	0.1	10	100		
Longitudinal Dispersivity v (for coupled models) (Layers 7 and 8, UFA, and Layer 10, MFA)	0.3	1	9	15	30	

Sensitivity Results

The sensitivity analyses were conducted for Kz, Kx and Ss using the uncoupled model with a grid size of 3,000 feet by 3,000 feet, and for dispersivity using the coupled model with a grid size of 12,000 feet by 12,000 feet. Both models were run on a weekly basis. After each sensitivity run, the average mean absolute error (MAE) was calculated for 64 monitor wells, and several average MAEs were graphed to show the sensitivity of the simulated heads to tested parameters with different multipliers in the model. Since the 64 monitor wells were installed in the primary aquifers, it is reasonably assumed that the average MAEs represent sensitivities of the model to tested parameters. **Figures 4-5**, **4-6**, and **4-7** showed the sensitivity of the simulated heads to vertical hydraulic conductivity (Kz), horizontal hydraulic conductivity (Kx), and specific storage (Ss) in the models, respectively. The average MAE at a multiplier of 1 showed the value for the calibrated model.

When comparing **Figures 4-5** through **4-7**, the simulated heads appear to be more sensitive to changes in the vertical hydraulic conductivity in confining units than the horizontal hydraulic conductivity and specific storage of the aquifers. As a result, increasing or decreasing the vertical hydraulic conductivity within the confining units resulted in larger average MAEs. It is seen in **Figure 4-5** that simulated heads were very sensitive to a lower Kz in Layer 2, which is the Tamiami aquifer and Upper Hawthorn confining unit connecting the surficial aquifer system (Layer 1, constant head boundary) and the Sandstone aquifer (Layer 3). When Kz was decreased by 0.1, the average MAE increased to around 5.3 feet, or approximately twice as much. This may be explained by the fact that recharge from surficial aquifer system is a major source of recharge to the Floridan aquifer system, especially in the northern portion of the model domain where the interaction between the two is greater and a larger surficial aquifer system driving head exists. This also indicates the importance of careful selection of Kz values for Layer 2, and more pilot points are needed to represent magnitudes and spatial distribution of Kz in the Lower Tamiami aquifer or its equivalent in the northern portion of the model. Variations in the Kz of the other confining units showed mixed results. In general, changes to Kz in the Middle Hawthorn and the Middle Floridan aquifer showed less response than modifications to Kz in the Lower Hawthorn and Lower Floridan aquitards.

From **Figure 4-6**, simulated heads were not very sensitive to changes of horizontal hydraulic conductivity in the primary aquifers. Increasing Kx caused a little decrease in average MAE in the UFA, MFA and Sandstone aquifer, and a slight increase was noted for the Mid-Hawthorn aquifer. When decreasing Kx, average MAE increased slightly for all aquifers. Simulated heads are not sensitive to changes in specific storage in MFA (Layer 10) (**Figure 4-7**). A decrease in the Ss of the UFA (Layers 7 and 8) caused larger average MAE changes but a corresponding increase in Ss for the same aquifer resulted in minimal changes to the global MAE.

Figure 4- 8 showed the sensitivities of simulated heads to global change in Kz, Kx and Ss in all simulated layers. Both an increase and decrease in the Kz values for all layers made the average MAE higher than the calibrated value. Decreases in Kx and Ss in all layers caused larger average MAEs but lower average MAEs as observed when the Kx and Ss was increased. Considering that the observed trends for parameters Kx and Ss correspond whether tested individually or globally, the calibrated values of Kx and Ss in the primary aquifers may be increased slightly on a global scale or in a single layer in order to generate smaller average MAE for simulated heads.

Figure 4-9 showed the sensitivities of simulated heads to changes of longitudinal dispersivities in UFA (Layers 7 and 8) and MFA (Layer 10). Simulated heads are not sensitive to increases of dispersivity in UFA; however, slight increases in average MAEs can be seen when dispersivities in the MFA increased. Simulated heads are more sensitive to changes of dispersivity in the MFA than the UFA, because the MFA is close to the Lower Floridan aquifer, defined as a constant head boundary with high solute concentrations. Changes of dispersivity affect solute transport in MFA and thus flow density and simulated heads. UFA is more or less insulated by both Upper Middle and Lower Middle confining units from the Lower Floridan aquifer.

Due to the complexity of LWCFAS Model, the calibrated model may be, to some extent, sensitive to uncertainties of other system or stress parameters. For example, the transient model may be sensitive to starting heads and solute concentrations that were generated from a quasi-steady-state model prior to the simulations, and any changes in heads and solute concentrations on model boundaries may also affect flow and solute transport close to model boundaries. Sensitivities of these parameters or values may be needed. In addition, incomplete historical pumping data may also introduce some uncertainties to the modeled system, and sensitivity analysis of simulated heads to changes in pumping data would be needed in this regard.

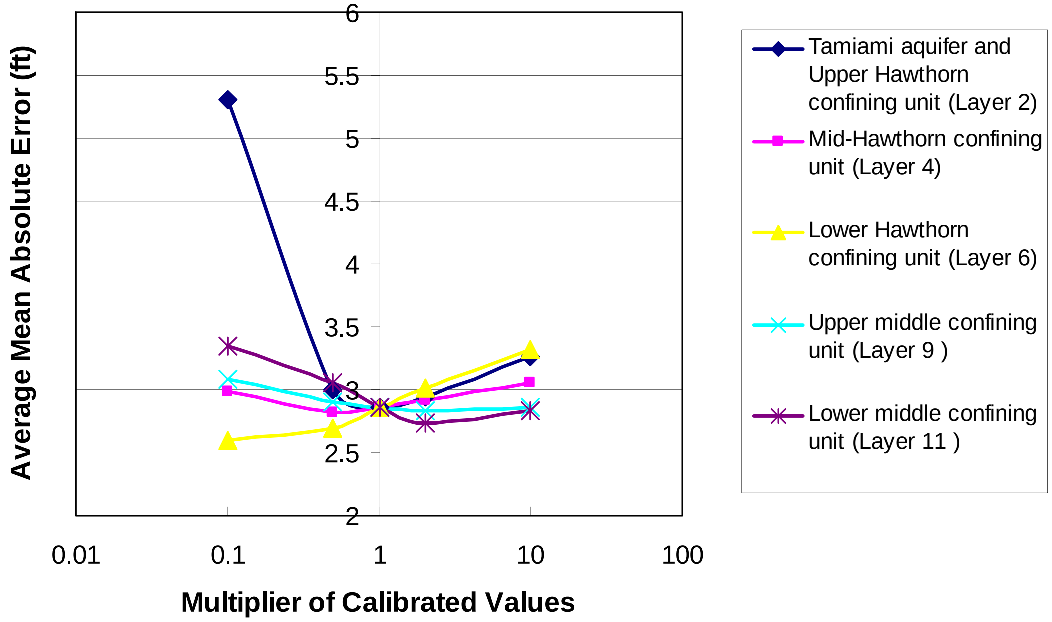

Figure 4-5. Sensitivity of simulated heads to changes in vertical hydraulic conductivity (Kz).

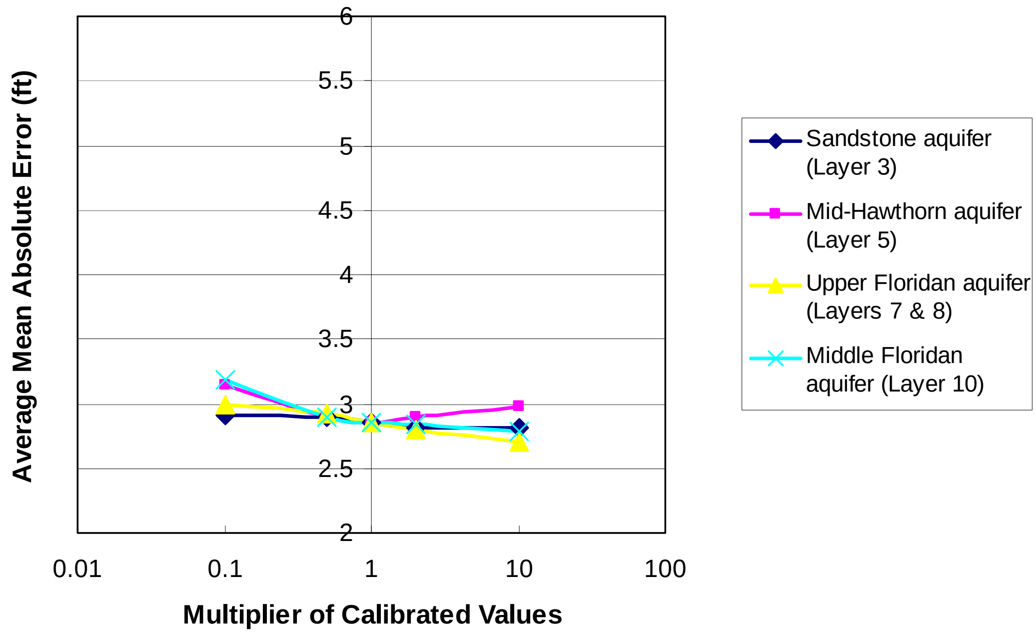

Figure 4-6. Sensitivity of simulated heads to changes in horizontal hydraulic conductivity (Kx) in major aquifers.

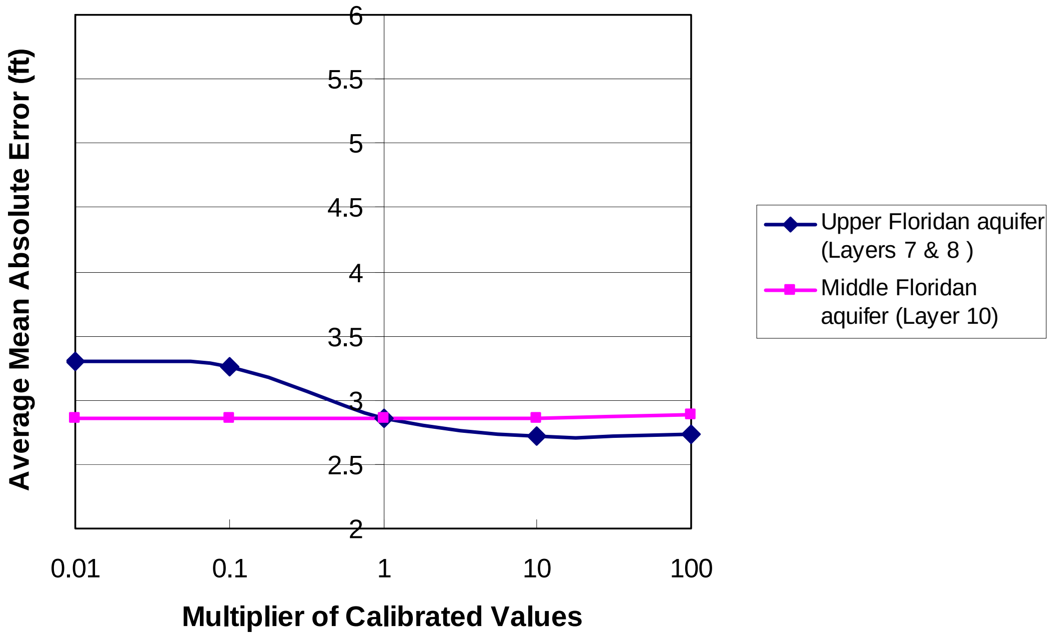

Figure 4-7. Sensitivity of simulated heads to changes in specific storage (Ss) in major aquifers.

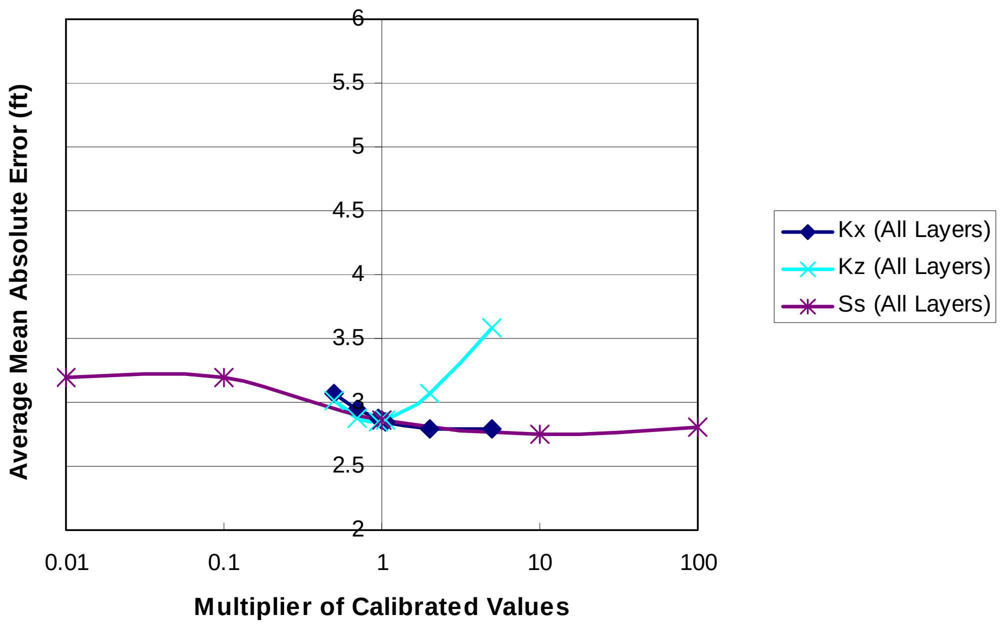

Figure 4- 8. Sensitivity of simulated heads to global changes in vertical hydraulic conductivity (Kz), horizontal hydraulic conductivity (Kx) and specific storage (Ss).

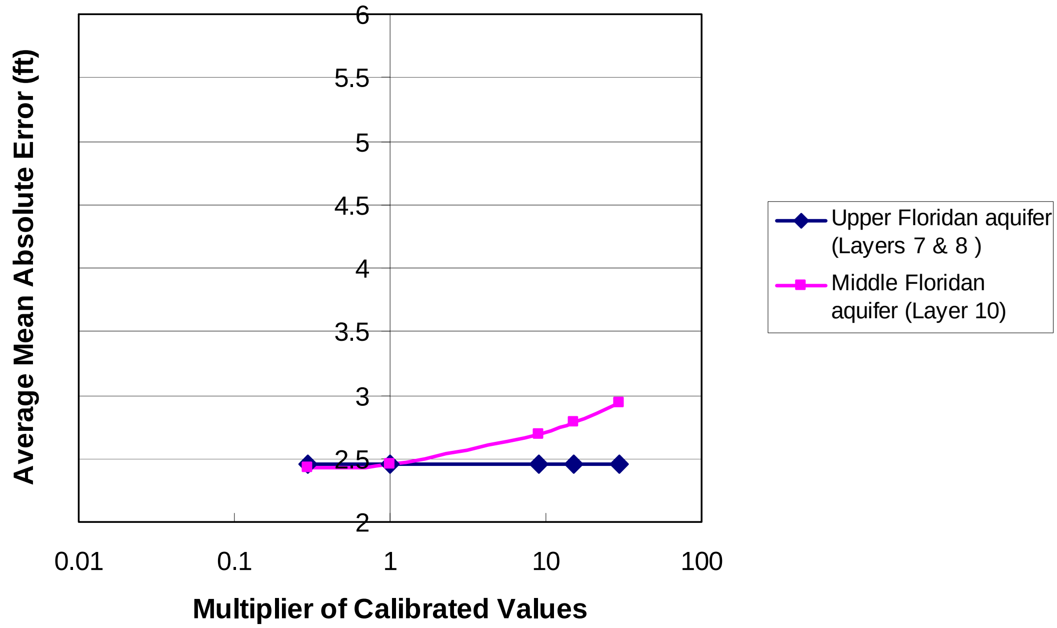

Figure 4-9. Sensitivity of simulated heads to changes in longitudinal dispersivities (v) in UFA and MFA.

CHAPTER 5
Conclusions and Recommendations

CONCLUSIONS

The Lower West Coast Floridan Aquifer System (LWCFAS) Model for the Intermediate and Floridan aquifer systems is based on a simplified representation of a complex, heterogeneous groundwater flow system. The governing equation used to solve the flow system is the density-dependent continuity equation derived from the principle of mass balance coupled with Darcy’s Law. This equation assumes that the flow is laminar and does not reach turbulent conditions. This is generally true throughout the study area, with the possible exception of flow near some major production wells or other areas of major stresses.

A model is any device that represents an approximation of a field situation (Anderson and Woessner 1992). As with all models, this one approximates reality, and as an approximation, has the potential to be continuously refined as new data and tools become available. There are areas of this model, both physical and conceptual, for which the approximation of reality is stronger or weaker than in others. These place limitations on the use of the model which has been noted in the documentation. Despite its limitations, however, there are a number of benefits to be derived from the LWCFAS Model. It can be used as a predictive tool for regional water supply planning, but its greatest value lies with the conceptual understanding of the flow system to be gained through the process of continual usage and refinement.

Based on the understanding gained through the model development and calibration process, the following observations on uses, advantages, limitations and general lessons learned from the model are offered:

- The model provides a three-dimensional density-dependent representation of the Lower West Coast (LWC) Planning Area with manageable run-times and numerical stability. As such, it is suitable tool for:
  - Long-term simulations
  - Regional-scale evaluations of potential saltwater intrusion issues, aquifer storage and recovery systems, and the effects of cumulative stresses on the aquifer system,
  - Conceptualization testing, and
  - Identifying data gaps

- Construction of the model using the UGEN/HBXY packages allows for changes in boundary conditions and pumping wells in a fraction of the usual time, and greatly reduces the files sizes on these input files.
- The model was developed in several different modes; 12,000 x 12,000 feet grid, and 3,000 x 3,000 feet grid, coupled and un-coupled flow and transport. There are advantages and disadvantages to running in each of these configurations. Having all available versions allows the user to choose the model most appropriate to its current simulation needs.
- The authors do not believe in over-fitting or manipulation of data to improve calibration. Consequently, the following issues limit confidence in the model calibration:
    - The quality of the groundwater withdrawal and injection information is imperfect.
    - The appropriateness of the coastal boundary is uncertain.
    - The inland boundary is based on only two or three wells, and values for some layers had to be estimated.
    - The head boundary within the Boulder zone is estimated
- Use of the model is also limited by its discretization, which assumes uniform hydraulic properties within a single cell. Flow within the Floridan aquifer system is best described as multiple, thin producing zones divided by thicker semi-confining units. Hydraulic property data, however, tends to be available only in terms of transmissivity across a larger thickness of these stacked producing / confining zones. The transmissivity data was divided by the total thickness of the hydrostratigraphic unit to produce initial hydraulic conductivity (K) estimates. These are average values, which tend to over-estimate K in the semi-confining units and under-estimate them within the producing intervals. As a result, simulated flow and transport rates may be underestimated because the semi-confining units tend to span larger sections of the aquifer system then the primary production zones.
- Significant simplification of aquifer properties was required to produce a regional-scale model capable of reasonable run times on currently available computer resources. To address the need for local-scale predictive simulations, models with finer horizontal discretization, and refined local hydrogeology would be required.
- Layer 2 of the model should not be used for prediction of hydrologic responses in the Lower Tamiami aquifer. The inland aquifer thickness and hydraulic properties are distorted to represent the aquifer system of comparable equivalence.

- The user should be aware that some layers of the model (Figures 23 to 28) may be considered to have 'highly deformed vertical discretization'. The MT3DMS manual warns that this can introduce numerical dispersion error, particularly in transport simulation. If transport is important to the simulation, the model should be run at the daily, rather than weekly time-step in order to minimize this dispersion.
- The present model does not simulate the temperature field and its effect on groundwater flow and transport. Previous investigators (e.g., Kohout 1965; Kohout et al. 1977) have suggested that temperature gradients may have a major effect on groundwater flow and transport in the FAS. Neglecting temperature, and thus potential variations to flow and transport in the aquifers (especially the Lower Floridan aquifer) may be a limitation for any FAS model.

RECOMMENDATIONS

- As more powerful computers become available, the vertical discretization of the model should be increased to allow for more refinement to improve solution of transport simulations.
- Calibration showed the model to be most sensitive to vertical conductance. This is a conceptual data gap within the region, and greater emphasis should be placed on the collection of this data.
- The LWCFAS Model was constructed using the best available data at the time, and for the given calibration period (1999–2001). Since that period, the SFWMD has added numerous monitor wells in the LWC that would greatly enhance the robustness of the model calibration. It is recommended that a second, post-2003 input data set be developed. The model should be validated, and if necessary, re-calibrated against this data-set.
    - Having valid boundary conditions is critical, particularly for very long simulations such as might be needed for long-term water supply modeling. To this end, the following is needed:
    - Additional water-level and chloride data are needed along the eastern boundary of the model.
    - Lower Floridan aquifer monitor wells are needed so that observed data from these wells can be used to refine the lower model boundary.

  - The coastal boundary is particularly important because of the proximity of the largest users to this boundary. Obviously the drilling of off-shore monitor wells to provide observed data is physically difficult, and most probably financially impossible. The District should explore all available technologies for field-truthing this boundary.

- Data from District monitor wells is not currently addressing the variability in the density of the water column in those wells, which affects the ability of end-users to obtain reliable equivalent piezometric heads. Additional monitoring protocols and quality control procedures should be emplaced to improve the usefulness of this data.

- The Lower Hawthorn and Suwannee producing zones of the Upper Floridan aquifer were simulated as a single unit (after Reese and Richardson 2007 in press). Hydraulically, there is little to separate these units, so there is some justification for this approach. Within the LWC Planning Area, however, more refined hydrostratigraphy would be advantageous. In Lee County, the combined thickness of the two units may exceed 800 feet, and the Lower Hawthorn zone tends to be significantly more permeable. Also, there are water withdrawals specifically targeting either of these two producing zones. As the model is enhanced, this modification to the hydrostratigraphy is recommended.

- Numerous recent publications and research (e.g., Rectenwald et al. 2008; Missimer and Maliva 2007; Reese and Richardson in press; Walker 2008) have begun to highlight the importance of fractures on flow within the FAS. This level of complexity in the hydrogeology is not represented in the current model, and the degree to which it should be is poorly understood. Is there preferential direction to anisotropy due to fracturing in the FAS? What is the impact of vertical fractures on confining units? Is the influence of fracturing evenly distributed through the region, or isolated to specific areas? These are questions that will need to be addressed before the movement of flow in the FAS can be fully understood.

- Within the specified limitations, the LWCFAS Model provides a useful tool for water management. It is intended as a dynamically evolving tool, which will both grow and improve with our understanding of the Floridan aquifer system, and lend itself to furthering that understanding.

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