Simulation of Submarine Ground Water Discharge to a Marine Estuary: Biscayne Bay, Florida

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Abstract

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Variable density ground water flow models are rarely used to estimate submarine ground water discharge because of limitations in computer speed, data availability, and availability of a simulation tool that can minimize numerical dispersion. This paper presents an application of the SEAWAT code, which is a combined version of MODFLOW and MT3D, to estimate rates of submarine ground water discharge to a coastal marine estuary. Discharge rates were estimated for Biscayne Bay, Florida, for the period from January 1989 to September 1998 using a three-dimensional, variable density ground water flow and transport model. Hydrologic stresses in the 10-layer model include recharge, evapotranspiration, ground water withdrawals from municipal wellfields, interactions with surface water (canals in urban areas and wetlands in the Everglades), boundary fluxes, and submarine ground water discharge to Biscayne Bay. The model was calibrated by matching ground water levels in monitoring wells, baseflow to canals, and the position of the 1995 salt water intrusion line. Results suggest that fresh submarine ground water discharge to Biscayne Bay may have exceeded surface water discharge during the 1989, 1990, and 1991 dry seasons, but the average discharge for the entire simulation period was only ~10% of the surface water discharge to the bay. Results from the model also suggest that tidal canals intercept fresh ground water that might otherwise have discharged directly to Biscayne Bay. This application demonstrates that regional scale variable density models are potentially useful tools for estimating rates of submarine ground water discharge.

Introduction

Kohout and Kolipinski (1967) demonstrated the ecological importance of submarine ground water discharge by showing that near-shore biological zonation in the shallow Biscayne Bay estuary was directly related to upward seepage of fresh ground water. Since then, most submarine ground water research has been motivated by the possibility that ground water discharge may be partially responsible for nutrient loading (Byrne 1999; Uchiyama et al. 2000; Masterson and Walter 2001) or pollutant contamination (Johannes 1980; Li et al. 1999) to coastal marine estuaries. For example, Corbett et al. (1999) used natural chemical tracers to identify areas in Florida Bay adjacent to the

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Florida Keys where ground water discharge may be causing nitrogen enrichment. These types of studies, which are extremely difficult in practice, provide explanations for water quality patterns that cannot be explained by more widely recognized processes such as rainfall or surface water runoff.

Corbett et al. (2001) use three categories to generalize the commonly used methods for measuring rates of submarine ground water discharge: (1) calculations using Darcy's law, (2) direct measurements with seepage meters, and (3) studies using natural or artificial tracers. Numerical ground water flow modeling is another method that can be used to estimate rates of submarine ground water discharge (Langevin 2001; Smith et al. 2001; Kaleris et al. 2002), but one that is not often used because of limitations in computer speed, data availability, and availability of a simulation tool that can minimize numerical dispersion. This paper provides an example of the types of results that can be obtained with a variable density ground water model and demonstrates the approach by presenting estimates of submarine ground water discharge rates to Biscayne Bay, Florida.

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Biscayne Bay is a coastal barrier island lagoon that relies on significant quantities of fresh water to sustain its estuarine ecosystem. During the past century, field observations have suggested that Biscayne Bay changed from a system largely controlled by widespread and continuous submarine discharge and overland sheetflow to one controlled by episodic discharge of surface water at the mouths of canals. Current ecosystem restoration efforts in southern Florida are examining alternative water management scenarios that could further change the quantity and timing of fresh water delivery to the bay. Ecosystem managers are concerned that these proposed modifications could adversely affect bay salinities. Currently, the two most important mechanisms for fresh water discharge to Biscayne Bay are thought to be canal discharges and submarine ground water discharge from the Biscayne Aquifer. Canal discharges are routinely measured and recorded, but few studies have attempted to quantify rates of submarine ground water discharge. As part of the Place-Based Studies Program, the U.S. Geological Survey (USGS) initiated a project in 1996 to quantify the rates of submarine ground water discharge to Biscayne Bay. This project was accomplished through field investigation and the development of a numerical ground water flow model that covers most of Miami-Dade County and parts of Broward and Monroe counties, Florida (Figure 1).

For the study of submarine ground water discharge to Biscayne Bay, project objectives and geometry of coastal hydrologic features required the development of a full three-dimensional model. This paper describes the model development and application of the variable density SEA-WAT code (Guo and Langevin 2002), a combined version of MODFLOW and MT3D, for the purpose of quantifying regional-scale submarine ground water discharge to a marine estuary. A detailed description of the USGS study is given in Langevin (2001).

Description of Study Area

The hydrology of southeastern Florida is characterized by the dynamic interaction between ground water and surface water. One of the most striking surface water features in southern Florida is the Everglades. North of the Tamiami Canal, the Everglades are divided into water conservation areas (Figure 1), which, although originally part of the continuous Everglades "river," are now separated by canals, highways, and levees. South of the Tamiami Canal, the Everglades are uncontrolled.

The physiographic features of southeastern Florida are relatively subtle, but because of the flat topography, small changes in land surface elevation can substantially affect surface and ground water flow. The Atlantic Coastal Ridge separates the Everglades from the Atlantic Ocean and Biscayne Bay. The ridge, which is 5 to 15 km wide, roughly parallels the coast in the northern half of Miami-Dade County. In southern Miami-Dade County, the Atlantic Coastal Ridge is located farther inland, and low-lying coastal areas and mangrove swamps adjoin Biscayne Bay. Prior to development, high-standing surface water in the Everglades flowed through the transverse glades (low-lying



Figure 1. Map of southern Florida showing location of study area, domain of regional scale model, and other hydrologic features. Extent of Atlantic Coastal Ridge modified from Parker et al. (1955).

areas that cut through the Atlantic Coastal Ridge) into Biscayne Bay.

Throughout much of the study area, a complex network of levees, canals, and control structures is used to manage the water resources. The major canals, operated and maintained by the South Florida Water Management District (SFWMD), are used to prevent low areas from flooding and to prevent salt water from intruding into the Biscayne Aquifer. These water management canals are particularly effective in managing the height of the water table because they were dredged into the highly transmissive Biscayne Aquifer. The sides of the canals are porous limestone, which means the canals are in direct hydraulic connection with the aquifer.

Beginning in the early 1900s, canals were constructed to lower the water table, increase the available land for agriculture, and provide flood protection. By the 1950s, excessive draining had lowered the water table 1 to 3 m and caused salt water intrusion, thus endangering the fresh water resources of the Biscayne Aquifer. In an effort to reverse and prevent salt water intrusion, control structures (Figure 1) were built within the canals near Biscayne Bay to raise inland water levels. On the western side of the coastal control structures, water levels can be 1 m higher than the tidal water level east of the structures.

Hydrostratigraphy

The hydrostratigraphy of southeastern Florida is characterized by the shallow surficial aquifer system and the deeper Floridan aquifer system. The work of Parker et al. (1955) and Kohout (1960) suggests that ground water discharging to Biscayne Bay originates from the Biscayne Aquifer, which is part of the surficial aquifer system. The highly permeable Biscayne Aquifer consists principally of porous limestone that ranges in age from Pliocene to Pleistocene. The vertical extent of the Biscayne Aquifer does not directly correlate with geologic contacts (Figure 2). Instead, the Biscayne Aquifer is defined by hydrogeologic properties. Fish (1988, p. 20) defines the Biscayne Aquifer as:

"that part of the surficial aquifer system in southeastern Florida comprised (from land surface downward) of the Pamlico Sand, Miami Oolite [Limestone], Anastasia Formation, Key Largo Limestone, and Fort Thompson Formation all of Pleistocene age, and contiguous highly permeable beds of the Tamiami Formation of Pliocene age, where at least 10 ft [3.05 m] of the section is highly permeable—a horizontal hydraulic conductivity of about 1,000 ft/d [305 m/d] or more."

The properties and extent of the Biscayne Aquifer in Miami-Dade County are presented in a report by Fish and Stewart (1991). They indicate that the aquifer is absent in much of western Miami-Dade County, but can be >55 m thick near the coast.

Coastal Ground Water Flow

Kohout (1960, 1964) studied coastal ground water flow by installing numerous monitoring wells along a transect perpendicular to the coast in the Cutler Ridge area (Figure 1; near Miami) in southeastern Florida. A cross section showing lines of equal chloride concentration for September 18, 1958, indicates that a tongue of relatively dense, saline ground water extended inland from the coast at the base of the Biscayne Aquifer (Figure 3). The cross section also shows that the interface between fresh ground water and saline water was a transition zone, rather than a sharp line. Kohout estimated that ~12.5% of the ground water discharged to Biscayne Bay was sea water that had been circulated through the aquifer, and that all submarine ground water discharge occurred within ~130 m of the shore.

Ground water flow to Biscayne Bay is affected by the water table elevation and the stage in the bay. Average values of daily and monthly stage for Biscayne Bay are shown in Figure 4. The average stage values were calculated using the downstream monitoring station at structure S-123 (Figure 1), which is located <1 km from the coast and near the central part of the study area. To ensure that the downstream stage values are not substantially affected by canal discharges or other potential influences, tide data from the Vir-



Figure 2. Geologic formations, aquifers, and semipermeable units of the surficial aquifer system across central Miami-Dade County (from Reese and Cunningham 2000). Section line shown on Figure 1.



Figure 3. Lines of equal chloride concentration for the Cutler Ridge area, September 18, 1958 (modified from Kohout 1964).

ginia Key station (Figure 1) was analyzed, and the records match. Figure 4 suggests that the stage of Biscayne Bay can significantly affect ground water discharge. Over a 12-month period, the average monthly stage of the bay can change by 0.6 m, as was the case in 1992. This is a significant change considering that the range in the water table elevations is ~3 m over the study area. Average daily stages and hourly stages also exhibit fluctuations up to 0.4 m, which can affect ground water discharge over shorter time periods.

Model Development

The regional scale model simulates transient ground water discharge to Biscayne Bay for a period from January 1989 to September 1998. The model was developed using the conceptual hydrologic model shown in Figure 5. It is assumed that the Biscayne Aquifer can be simulated with an equivalent porous medium (EPM). Historical observations suggest that submerged ground water springs were once active within Biscayne Bay. By using the assumption of an EPM, individual springs and conduits are not explicitly simulated, but rather the properties of the conduits are averaged within model cells. This assumption limits the interpretation of model results at local scales, but is thought to be appropriate when conduits or fractures are much smaller than the scale of the model.





Figure 5. Conceptual hydrologic model used to develop numerical models of ground water flow.

Governing Equations

Variable density ground water flow is described by the following partial differential equation:

$$\nabla \cdot \rho K_f \left(\nabla h_f + \frac{(\rho - \rho_f)}{\rho_f} \nabla z \right) = \rho S_f \frac{\partial h_f}{\partial t}$$
$$n \frac{\partial \rho}{\partial C} \frac{\partial C}{\partial t} - \overline{\rho q} \tag{1}$$

where

x, *y*, and *z* are coordinate directions where *z* is aligned with gravity [L].

 ρ is fluid density [ML⁻³].

- K_f is the equivalent fresh water hydraulic conductivity [LT⁻¹].
- h_f is the equivalent fresh water head [L].
- ρ_{f} is the density of fresh water [ML⁻³].
- \vec{S}_{f} is equivalent fresh water storage coefficient [L⁻¹].

t is time [T].

- *n* is porosity $[L^0]$.
- *C* is the concentration of the dissolved constituent that affects fluid density $[ML^{-3}]$.
- $\overline{\rho}$ is the fluid density of a source or sink [ML⁻³].
- \overline{q} is the flow rate of the source or sink [T⁻¹].

To solve the variable density ground water flow equation, the solute-transport equation also must be solved because fluid density is a function of solute concentration, and concentration may change in response to the ground water flow field. For dissolved constituents that are conservative, such as those found in sea water, the solute transport equation is

$$\frac{\partial C}{\partial t} = \nabla \cdot (D\nabla C) - \nabla \cdot (vC) - \frac{q_s}{n}C_s \qquad (2)$$

where

D is the dispersion coefficient $[L^2T^{-1}]$. *v* is the ground water flow velocity $[LT^{-1}]$. q_s is the flux of a source or sink $[T^{-1}]$.

 $C_{\rm s}$ is the concentration of the source or sink [ML⁻³].

Simulation Code

The original SEAWAT code was written by Guo and Bennett (1998) to simulate ground water flow and salt water intrusion in coastal environments. SEAWAT uses a modified version of MODFLOW (McDonald and Harbaugh 1988) to solve the variable density, ground water flow equation (Equation 1) and MT3D (Zheng 1990) to solve the solute-transport equation (Equation 2). To minimize complexity and runtimes, the SEAWAT code uses a one-step lag between solutions of flow and transport. This means that MT3D runs for a time step, and then MODFLOW runs for the same time step using the last concentrations from MT3D to calculate the density terms in the flow equation. For the next time step, velocities from the current MOD-FLOW solution are used by MT3D to solve the transport equation. For most simulations, the one-step lag does not introduce significant error, and the error can be reduced or evaluated by decreasing the length of the time step.

One major reason the SEAWAT code was selected for this study is that it uses MT3D to solve the transport equation. MT3D contains a variety of methods for solving the transport equation including the method of characteristics (MOC). During the simulation of solute transport, numerical dispersion and other problems (long computer runtimes, temporal and spatial resolution requirements, etc.) often are encountered. With SEAWAT, an acceptable solution can usually be obtained because MT3D has a variety of solution techniques, including MOC, which is ideal for reducing numerical dispersion. For the simulations presented in this paper, MOC was used with 16 to 256 particles per cell.

Another advantage of using SEAWAT is that it uses two widely accepted modeling codes: MODFLOW and MT3D, which means that SEAWAT is modular and contains the "package" approach for including various boundary conditions and transport options. As a result, SEAWAT contains packages, such as the drain and river, which are conceptually similar to the equivalent packages in MODFLOW. In addition, SEAWAT reads and writes standard MODFLOW and MT3D data files, which are easily manipulated with commercially available pre- and post-processors.

The original SEAWAT code (Guo and Bennett 1998), referred to as version 1, was modified for this study of Biscayne Bay. Langevin and Guo (1999) and Langevin (2001) present a description of those modifications. Guo and Langevin (2002) present the formal documentation for version 2 of the SEAWAT code, which was released by the U.S. Geological Survey after the completion of the Biscayne Bay study. Version 2 contains a newer version of MT3D (Zheng and Wang 1998) and is distributed within the public domain.

Spatial and Temporal Discretization

To simulate ground water flow to Biscayne Bay, a regularly spaced, finite-difference model grid was constructed and rotated so that the y-axis would roughly parallel the coast (Figure 6). Each cell is $1000 \text{ m} \times 1000 \text{ m}$ in the horizontal plane. The grid consists of 89 rows and 71 columns, and the rotation angle from true north is clockwise 14 degrees. The purpose for rotating the grid is to align model rows with the principal direction of ground water flow, which is primarily toward Biscayne Bay. When ground water flow is not parallel to one of the primary model axes, some numerical schemes can experience accuracy problems in the solution to the transport equation. Another reason for rotating the model grid is that future modifications to the model may require a higher level of discretization at the coast. A rotated model grid allows the resolution along a flow line to be increased by dividing columns near the coast. To maintain reasonable computer runtimes, the domain of the regional model was not extended south to Florida Bay. Future versions of the model, however, may extend into Florida Bay as a method for eliminating potential boundary effects.

Accurate simulation of variable density flow systems requires a finer vertical resolution compared to that required for simulating constant density flow systems. This increased resolution is necessary because of transport considerations and because vertical density gradients must be



Figure 6. Finite-difference grid and boundary conditions in the upper layer for the regional scale ground water flow model in southern Florida.

resolved in order to calculate accurate flow velocities. Accordingly, the model grid, which represents the Biscayne Aquifer, consists of 10 layers-more layers than would be required for a typical ground water flow model that does not represent density variations. The top elevation of layer 1 is spatially variable and corresponds with land surface elevation, based on a compiled topographic contour map provided by Everglades National Park. For model cells within Biscayne Bay, the top of layer 1 has a value of 0.0 m. The bottom of layer 1 is set at an elevation of 5.0 m below sea level. To minimize the effects of numerical problems that can occur in solute-transport models, the grid was designed so that layers would be flat and cells would have a uniform volume (1000 m \times 1000 m \times 5 m). Although the volume for each model cell in layer 1 may be slightly variable because of the variation in land surface elevation, model cells in layers 2 through 10 have a uniform thickness of 5 m, and thus a uniform cell volume. The bottom elevation for layer 10 is 50 m below sea level. The base of the Biscayne Aquifer, as defined by Fish and Stewart (1991), generally slopes from west to east. This variability in aquifer thickness was included in the model by inactivating model cells with cell centers below the base of the Biscayne Aquifer.

The nearly 10-year simulation period is divided into 116 monthly stress periods. For each stress period, the average hydrologic conditions for that month are assumed to remain constant. This means that the model does not simulate hourly or daily hydrologic variations, but rather seasonal and yearly variations. Further temporal discretization is introduced in the form of time steps within each stress period. Each stress period is divided into one or more time steps, the lengths of which are determined by SEAWAT to meet specified criteria associated with solving the solutetransport equation. For the regional scale model, about 20 time steps were required for each stress period.

Assignment of Aquifer Parameters

The approach for assigning aquifer parameters that pertain to ground water flow-and-solute transport was to use the simplest distribution that would result in adequate representation of the flow system. Parameter values used in the model are listed in Table 1. Langevin (2001) provides a detailed description of how aquifer parameters were determined.

Boundary Conditions

The boundary conditions available in SEAWAT consist of those packages released with the 1988 version of MODFLOW and the time variant constant-head package. Methods for generating boundary conditions for the regional model follow the standard approaches outlined by Anderson and Woessner (1992) and Zheng and Bennett (2002). Table 2 provides a summary of the boundary conditions, which are discussed in detail by Langevin (2001). A description of the Biscayne Bay boundary condition is provided as follows.

The model cells in layer 1 representing Biscayne Bay were simulated with the time varying constant head (CHD) package in SEAWAT. By specifying a constant fresh water head boundary in layer 1, the elevation for the bottom of Biscayne Bay corresponds to the center elevation of layer 1; thus, the simulated bay bottom is flat with an elevation of 2.5 m. Average monthly values (Figure 4) for downstream stage at structure S-123 were used to set the water level in the constant-head cells. The downstream stage measurement at structure S-123 was used because this structure is located at the coast and lies near the center of the Biscayne Bay shoreline. Results from a calibrated hydrodynamic circulation model, which covers all but the northernmost part of Biscayne Bay, suggest that the salinity in the bay is temporally and spatially variable because of surface water discharge (Wang 2001). Results from the circulation model were used to set spatially varying and temporally varying concentration values for the constant concentration and constant-head cells representing Biscayne Bay. The few data that exist for the northern part of Biscayne Bay suggest that salinity for the northern area may be lower than that of sea water; however, a constant value of 35 kg/m³ was spec-

Parameter Description	Comment
Hydraulic conductivity (m/d)	
Zone 1 ¹ : $K_h = 9000$ $K_v = 90$	Value used in calibrated flow model by Merritt (1996) to represent Miami Limestone, Fort Thompson, and permeable zones of the Tamiami Formation
Zone 2 ¹ : $K_h = 3$ $K_v = 0.3$	Value assigned to represent peat and marl units in the upper part of the Biscayne Aquifer
Zone 3 ¹ : $K_{h} = 1500$ $K_{v} = 15$	Value assigned by Merritt (1996) to match flow and head patterns near central Biscayne Bay
Primary and secondary storage coefficient ² (unitless)	
Layer 1: $SF1 = 1.0$ SF2 = 0.2	Primary coefficient used for infrequent case when water table rises above land surface; secondary value equal to specific yield estimated by Merritt (1996)
Layers 2–10: $SF1 = 5.9 \times 10^{-5}$ SF2 = 0.2	Primary coefficient estimated using compressibility for fractured rock $(2 \times 10^{-10} \text{ m}^2/\text{N})$; Domenico and Schwartz 1990, p. 111); secondary value equal to specific yield estimated by Merritt (1996)
Porosity (unitless)	
Uniform value: n = 0.2	Assumed porosity of porous limestone similar to specific yield estimated by Merritt (1996)
Dispersivity (m)	
Uniform values: $\alpha_{\rm L} = 5.0$ $\alpha_{\rm T} = 0.5$	Dispersivity values determined through calibration of two cross-section models with fine horizontal and vertical resolution (Langevin 2001)

²Primary storage coefficient used by the model when head is above top elevation of cell; secondary storage coefficient used when water table located within cell (McDonald and Harbaugh 1988)

Note: K_h , horizontal hydraulic conductivity; K_v , vertical hydraulic conductivity; SF1, primary storage coefficient; SF2, secondary storage coefficient; n, porosity; α_r , longitudinal dispersivity; α_r , transverse dispersivity

Table 2 Boundary Conditions Used in Regional Scale Ground Water Flow and Transport Model

Boundary Description	Boundary Type	Comments
Model perimeter		
Active inland cells, layers 1–10	GHB	Time varying equivalent fresh water head value estimated from water table TINs ¹ and salinity estimates
Active offshore cells, layers 1-10	CHD	Time varying equivalent fresh water head calculated from Biscayne Bay stage and salinity
Base of model		Disedjile Daj slage and samnej
Base of Biscayne Aquifer	No-flow	Model cells with center elevation below base of Biscayne Aquifer were inactivated; similar approach used by Merritt (1996) and Swain et al. (1996)
Biscayne Bay		
North Biscayne Bay	CHD	Time varying equivalent fresh water head calculated from Biscayne Bay stage and salinity value of 35 kg/m^3
Central and South Biscayne Bay	CHD	Time varying equivalent fresh water head calculated from Biscayne Bay stage and salinity from hydrodynamic model (Wang 2001)
Canals		
Primary water management canals and selected secondary canals (Figure 6)	RIV	Canal stages vary temporarily based on field data; conductance calculated using formation by Swain et al. (1996) and by calibration
Standing surface water		
Everglades and coastal wetlands (Figure 6)	GHB	Time varying heads calculated using water table TINs ¹ and salt concentration of zero; conductance value of 1×10^5 m ² /d determined by calibration
Recharge		
Uppermost active cell	RCH	Recharge concentration assigned value of zero; recharge rate estimated from rainfall and runoff based on method described by Restrepo et al. (1992)
Evapotranspiration		
Uppermost active cell	EVT	Evapotranspiration rate assigned based on Merritt (1996); extinc- tion depths range between 0.15 and 1.8 m based on Restrepo et al. (1992)
Ground water withdrawals		
Municipal wellfields	WEL	Monthly withdrawals for each wellfield were obtained from South Florida Water Management District (1999) and from Goldenberg (1999)

¹For each month of the simulation, triangular irregular networks (TINs) were developed for the water table using available surface water and shallow ground water monitoring stations.

Note: GHB, general head boundary; CHD, time variant constant head; RIV, river; RCH, recharge; EVT, evapotranspiration; WEL, well

ified for the part of Biscayne Bay not covered by the circulation model. The model results from Wang (2001) suggest that the salinity of central Biscayne Bay ranges from ~15 to 35 kg/m^3 at the shoreline, 20 to 35 kg/m^3 at a distance of 5500 m from the shoreline, and 25 to 35 kg/m^3 at a distance of 13,500 m from the shoreline. In the circulation model, the larger fluctuation in salinity near the coast is primarily due to significant fresh water discharges at canal mouths.

Initial Conditions

Initial water levels were specified for the model by interpolating values from a two-dimensional representation of the water table surface for January 1989. For most modeling applications, the use of field data to specify initial water levels can introduce model error at the beginning of the simulation; however, for the highly permeable Biscayne Aquifer, numerical experiments have shown that errors introduced by specifying initial water levels with field data are eliminated several weeks into the simulation. Early attempts to specify initial concentrations consisted of running the model over and over until the position of the interface reached dynamic equilibrium. The position of the interface at dynamic equilibrium, however, was too far inland for the northern part of the model. Due to the lowering of the water table beginning in the early 1900s, the interface position may not be at equilibrium. Thus, the dynamic equilibrium approach for setting initial concentrations was replaced with a hybrid method developed by trial and error. Later attempts to set initial concentrations used the 1995 salt water intrusion line by Sonenshein (1997), who delineated the position of the interface at the base of the Biscayne Aquifer using chloride concentrations from monitoring wells and time-domain electromagnetic soundings. The first attempt with the 1995 salt water intrusion line, which is nearly identical to the 1984 salt water intrusion line mapped by Klein and Waller (1985), consisted of specifying sea water concentrations (35 kg/m³) east of the line and fresh water concentrations west of the salt water intrusion line. This procedure for specifying initial concentrations was used for each layer and resulted in a vertical wall of sea water at the 1995 salt water intrusion line.

Results from early simulations suggested that a better estimate for initial salinity concentrations would reduce the length of simulation time required to achieve a stable position for the salt water interface, thus increasing the length of time model results would be unaffected by the initial salinity distribution. The initial salinity distribution was improved by linearly interpolating concentrations between the 1995 salt water intrusion line and Biscayne Bay. The initial salinity distribution was further improved by incorporating the results from an airborne geophysical survey (Fitterman and Deszcz-Pan 1998) of the southern part of the model area.

Model Calibration

The regional scale model was calibrated using trial and error by matching heads, ground water exchange rates with canals, and position of the salt water interface. The mean error (ME) in head for all stress periods and wells (6525 values in total) is 0.08 m. The positive value for ME indicates that simulated values of head generally are higher than observed values of head. The mean absolute error (MAE) is 0.15 m, which is an acceptable value considering that observed heads range from -2.23 to 2.51 m. This means that the MAE relative to the range in observed heads is ~3%. The root mean square error (RMSE) is 0.27 m, indicating that ~68% of the head differences are within ± 0.27 m of the ME. A histogram constructed from the differences between observed and simulated heads suggests that the differences are normally distributed with a mode of ~0.05 m. Langevin (2001) presents a more thorough comparison of observed versus simulated water levels.

Calibration of the regional scale model to canal baseflow was performed for surface water basins (Cooper and Lane 1987) with measured surface water inflows and outflows. For each of these basins, simulated baseflow was combined with the total runoff value estimated from the land-use method described earlier. This combined value was then compared with the net canal loss or gain measured for the basin. Net losses and gains were calculated for the selected surface water basins by subtracting canal inflows from canal outflows. It is assumed that the difference between inflow and outflow is equal to baseflow and runoff. The mathematical equation is:

baseflow + runoff = canal outflow - canal inflow

where the left side of the equation is based on the simulation and the right side is based on measured quantities. The flow terms on the right side of the equation, originally calculated from rating curves at structures, were obtained from the database of the SFWMD. Canal outflow is the sum of all surface water discharge that flows out of the surface water basin. Canal inflow is the sum of all surface water discharge that flows into the surface water basin. This approach assumes that direct rainfall to a canal, direct evaporation from a canal, and storage within a canal are negligible. For the 12 surface water basins used in the calibration, the mean absolute error between observed and simulated baseflow and runoff ranges between 1.9×10^5 and 5.5×10^5 m³/day. The mean difference between measured canal outflow and canal inflow, combined for the 12 surface water basins, is $3.1 \times 10^6 \text{ m}^3/\text{day}.$

For the regional scale model to accurately simulate the discharge of ground water to Biscayne Bay, the model must accurately simulate the three-dimensional distribution of ground water salinity. Unfortunately, data are lacking to adequately characterize the three-dimensional distribution of ground water salinity because most monitoring wells are installed near the toe of the salt water interface rather than within the transition zone. Rather than compare the few point measurements of ground water salinity with simulated values of salinity, model results are reduced to two dimensions to facilitate a comparison with the 1995 position of the salt water intrusion line (Sonenshein 1997). In Figure 7, the simulated salt concentrations in the lowermost active model cell (the base of the Biscayne Aquifer) are shaded according to their corresponding salinity values.

In general, the model reasonably approximates the location of the interface between fresh water and salt water except for the area north of the Miami Canal (Figure 7). In this area, the simulated position of the interface is located too far inland by ~6 to 8 km. In the central and southern portion of the model, the simulated interface appears to be within one or two model cells of the position mapped by Sonenshein (1997). The saline ground water at the southwestern corner of the model represents the inland extent of intrusion from Florida Bay. Simulated salinities in this area are relatively high because the concentrations assigned to the general head boundaries were inferred from an airborne geophysical survey.



Figure 7. Simulated values of ground water salinity at the base of the Biscayne Aquifer compared with the 1995 salt water intrusion line.

There are several possible explanations for the discrepancy in the northern part of the model. First, the simulated ground water heads in this area may be too low, which is the case for one of the coastal monitoring wells in this area. Simulated heads that are too low may have been caused by a lack of sufficient head data that resulted in assignment of inappropriate aquifer parameters or hydrologic stresses, such as recharge or evapotranspiration. Another possible explanation for the poor match north of Miami Canal is that the model may not accurately represent the process of dispersion in this area. Konikow and Reilly (1999) discuss the rationale behind the concept that dispersion prevents the interface from moving inland in north Miami-Dade County to a position predicted by the Ghyben-Herzberg principle. Thus, if the model does not simulate enough dispersion, the simulated interface will be located too far inland. A third possible explanation for the poor match is that the boundary condition used to represent Biscayne Bay may not be set appropriately. In the model, an equivalent fresh water head value was calculated for the constant-head cells representing Biscavne Bay using the density of sea water (1025 kg/m^3). Thus, if the actual density of north Biscayne Bay was less than sea water, the equivalent fresh water head would be lower, and the interface would not move as far inland. Additional research is necessary to determine which of these explanations, or combination of explanations, is most likely.

Simulated Estimates of Submarine Ground Water Discharge to Biscayne Bay

The simulated ground water flow from the active model cells into the coastal constant-head cells is assumed to represent the discharge of ground water to Biscayne Bay. In addition to simulating the volumetric flow rate, the model also simulates the salt concentration of the ground water flow into the constant-head cells. This salt concentration is assumed to represent the salinity of the ground water that discharges to Biscayne Bay. The simulated salinity of ground water discharge to Biscayne Bay ranges from nearly fresh at the shoreline to nearly sea water some distance offshore. To simplify the results, simulated discharge estimates are presented as the fresh water portion of the total discharge. The fresh water portion of the ground water discharge is calculated from the total discharge using the following equation:

$$Q_f = Q_T \frac{(\rho_s - \rho)}{(\rho_s - \rho_f)} \tag{3}$$

where:

 Q_f is simulated fresh ground water discharge, in m³/day. Q_T is simulated total ground water discharge, in m³/day. ρ_s is fluid density of sea water, in kg/m³. ρ is simulated fluid density of ground water discharging to

Biscayne Bay, in kg/m³.

When the fluid density of the ground water discharge is equal to 1000 kg/m³, the fresh ground water discharge is equal to the total ground water discharge. When the fluid density of the ground water discharge is equal to the fluid

density of sea water (1025 kg/m³), the fresh ground water discharge is equal to zero. During certain times, simulated flow is from the bay into the aquifer. When this condition occurs, Q_T is negative, but Q_f is zero. A subroutine was added to SEAWAT to calculate and sum the Q_T and Q_f terms between each constant-head cell and the adjacent active cells. These flow terms are written to a file following each time step. At the end of a model run, a post-processing routine calculates the average flows for each constant-head cell by stress period.

One potential problem with calculating fresh ground water discharge estimates from simulated density is that the resulting fresh water discharge quantities are directly dependent on salt concentrations. (Density is a linear function of salt concentration.) As previously mentioned, ground water salinities are considered calibrated when the simulated position of the salt water toe matches with the observed position. This does not ensure that the simulated salt concentrations are calibrated. The average salt concentration of simulated discharge to Biscayne Bay is about half that of sea water, and thus half of the total discharge is fresh water. This suggests that if salt concentrations were in error by 100% (17.5 kg/m³), estimates of fresh ground water discharge might be in error by about a factor of two.

Results from the regional scale model indicate that fresh and brackish ground water discharges to Biscayne Bay along the coastline and into the tidal portions of the Miami, Coral Gables, and Snapper Creek Canals (locations shown in Figure 1). The model suggests that fresh ground water discharge at the coastline of Biscayne Bay is similar in magnitude to the fresh ground water discharge to tidal canals. The average rate of fresh ground water discharge is $\sim 3.7 \times 10^5 \,\mathrm{m^3/day}$ for the coastline of Biscayne Bay, about 1.8×10^5 m³/day for the tidal portion of the Miami Canal, $\sim 1.4 \times 10^5$ m³/day for the tidal portion of the Coral Gables Canal, and $\sim 3.4 \times 10^4 \text{ m}^3/\text{day}$ for the tidal portion of the Snapper Creek Canal. The annual fluctuation in fresh ground water discharge is $\sim 1 \times 10^5 \text{ m}^3/\text{day}$ for the coastline of Biscayne Bay and the tidal portions of the Miami and Coral Gables Canals, and $\sim 3 \times 10^4 \, \text{m}^3$ /day for the tidal portion of the Snapper Creek Canal. Fluctuations in ground water discharge appear to be dampened because sea level was highest during the wet season when the water table was relatively high and lowest during the dry season when the water table was relatively low.

A comparison was made between simulated fresh ground water discharge and measured surface water discharge from the coastal control structures. Based on the results for the simulation period (1989–1998), fresh ground water discharge seems to be an important mechanism of fresh water delivery to Biscayne Bay during some dry seasons (Figure 8). For the dry seasons of 1989, 1990, and 1991, model results suggest that fresh ground water discharge exceeded the surface water discharge to Biscayne Bay. During the wet season, however, fresh ground water discharge is about an order of magnitude less than the surface water discharge. For the total simulation period, ground water discharge, or 2% of annual rainfall over the active model domain.



Figure 8. Simulated rates of fresh ground water discharge compared with measured rate of surface water discharge to Biscayne Bay.

Nearly 100% of the fresh ground water discharge to Biscayne Bay is to the northern half of the bay, north of structure S–123 (Figure 1). South of structure S–123 (Figure 1), where land surface elevations are <1 m above sea level, the water table was unable to develop enough head to drive ground water discharge into the bay. In this area, evapotranspiration from coastal wetlands is the dominant hydrologic process. If simulated salinities for the northern part of the model were improved, there may be even higher rates of fresh submarine ground water discharge to the northern half of Biscayne Bay.

Sensitivity to Biscayne Bay Boundary Condition

By using the specified concentration boundary condition (also referred to as Type I or Dirichlet boundary) for Biscayne Bay, solute enters the active aquifer domain through advection and dispersion. This type of boundary condition was selected to represent Biscayne Bay because the model uses monthly stress periods; therefore, dispersion beneath Biscayne Bay as a result of tidal and daily fluctuations in stage was not directly included in the model. It was assumed that the dispersion caused by these relatively high frequency variations in stage could be represented with the dispersive salt flux that results from using the constant concentration boundary condition. There was, however, no direct evidence to support the selection of this type of boundary condition for solute transport, nor was there an adequate method for assigning an appropriate dispersion coefficient or dispersivity value. A mixed condition (Type III or Cauchy boundary) is another boundary type available in SEAWAT and can be used with a constant-head boundary (Zheng and Bennett 2002). With the mixed-boundary condition in SEAWAT, inflow from the boundary is assigned a user-specified concentration, whereas outflow to the boundary carries the concentration calculated at the active cell adjacent to the boundary. Regardless of the flow direction, the concentration gradient is held at zero, which eliminates the dispersive flux across the boundary. The following sensitivity analysis was performed to evaluate the effects of boundary type on discharge rates to Biscayne Bay.

To evaluate the effects of solute-transport boundary type on simulated rates of fresh ground water discharge, another simulation was run in which a mixed boundary was specified with concentration values from the circulation model. By using a mixed boundary rather than holding the concentration constant, salt mass enters the active aquifer domain only through advection. For this simulation, the average rate of fresh ground water discharge directly to Biscayne Bay is 5.8 imes 10⁵ m³/day, or 55% more than for the simulation with a constant concentration boundary (referred to as the base case). The reason that the rate of fresh ground water discharge is 55% more for this simulation is because the simulated salt concentrations beneath the bay are less than the simulated concentrations in the base case. With the constant concentration boundary, salt mass enters through advection and dispersion, causing simulated concentrations to be relatively high beneath the bay (as in the base case). Therefore, the fresh ground water discharge, which is calculated from the actual discharge and the discharge concentration, tends to be larger with a mixed boundary. One possible method for reducing the quantity of salt mass that enters the aquifer from a constant concentration boundary by dispersion is to lower the dispersivity values near the boundary.

The effects of bay salinity on ground water discharge were evaluated by running a simulation in which a salinity value of 35 kg/m³ was specified for the entire bay, a simplified assumption that was originally used in the model development. For this case, the average rate of simulated fresh ground water discharge directly to Biscayne Bay is 2.2 \times $10^5 \text{ m}^3/\text{day}$, ~40% less than for the base case. This rate is less than the base case for two reasons: First, the equivalent fresh water head value assigned to the constant-head cells is higher because the density of the bay water is higher. Second, in the base case, a portion of the "fresh" discharge may actually be brackish water that entered the aquifer from Biscayne Bay rather than from inland recharge. When the concentration is fixed at 35 kg/m³, this extra source of partially fresh bay water is eliminated, and salt concentrations beneath the bay are higher. The result is a lower calculated flux of fresh discharge to the bay.

Another simulation also was run with the salinity value of 35 kg/m³ used with the mixed boundary type. For this case, the average rate of simulated fresh ground water discharge directly to Biscayne Bay is 4.9×10^5 m³/day, ~30% more than the rate simulated with the base case. Based on this comparison, the boundary type seems to affect the fresh discharge rates more than the salinity values used to represent the bay.

These sensitivity simulations illustrate the importance of the boundary condition used to represent a marine estuary. Because the quantity of fresh ground water discharge depends on the solute concentrations adjacent to and beneath the estuary, slight variations in the boundary-condition type and the specified concentration value can have a large effect on the simulated rate. For the Biscayne Bay model, the use of a specified concentration boundary results in less fresh ground water discharge compared to a similar model that uses a mixed boundary. Additionally, the model results suggest that fresh ground water discharge rates are sensitive to the salinity of the estuary. Fresh discharge rates tend to increase when the salinity of the estuary decreases.

Sensitivity of Fresh Discharge to Horizontal Grid Resolution

An analysis was performed to evaluate the sensitivity of simulated submarine ground water discharge estimates to horizontal grid resolution. Rather than perform the analysis with the three-dimensional regional model, which would require unreasonably long simulation times, a simple cross section model was developed using representative Biscayne Aquifer parameters (Figure 9). A head-dependent boundary (GHB) was used as the inland boundary, as opposed to a specified flux, so the net fresh water flux to the bay would be calculated by the model rather than specified as input. Fresh ground water enters from the GHB cells, flows toward the coast, and discharges into the constant head cells. A flux of sea water into the aquifer is required from some of the constant-head cells to provide a source of salt for the brackish ground water that discharges into the constant-head cells.

Seven simulations were performed, each with different horizontal grid spacing within the transition zone. In the grid design for each simulation, the horizontal node spacing between adjacent cells did not vary by more than a factor of 1.5. Simulations were run until steady-state flow and transport conditions were achieved (~10,000 days). Table 3 lists the rates of simulated fresh water inflows from the generalhead boundary and sea water inflows from the constanthead boundary. Rates are expressed as m3/day per meter of shoreline, or m²/day. The analysis suggests that, for the case tested, the rate of fresh submarine ground water discharge to the constant-head cells does not significantly depend on the horizontal grid spacing. Salinity contours for the seven simulations (not shown) also were identical, except in the upper layers near the constant-head boundary. The fresh discharge estimate with 1000 m grid resolution (resolution used in regional model) is only ~7% less than the simulated estimate from the model with 31.25 m resolution. The rate of circulated sea water, however, is highly dependent on

Table 3Results from Sensitivity Analysis of FreshSubmarine Discharge to Horizontal Grid Spacing

Horizontal Grid Spacing	Fresh Water Inflow from GHB Cells (m²/d)	Seawater Inflow from Constant Head Cells (m ² /d)
2000	4.33	1.25
1000^{1}	4.62	3.02
500	4.84	7.08
250	4.90	10.78
125	4.93	13.84
62.5	4.93	15.05
31.25	4.95	15.93

horizontal grid resolution. As grid spacing decreases from 1000 to 31.25 m, the total flux of sea water through the system increases by a factor of five. This means that more refined models may be required if simulated discharge rates are compared with the total brackish water flux measured with seepage meters.

Discussion and Conclusions

Regional scale simulation of variable density ground water flow is rarely performed in three dimensions because of limitations in computer speed, data availability, and availability of a simulation tool that can minimize numerical dispersion. The development and application of the regional scale model presented in this paper suggests that large-scale simulation of variable density ground water flow is a viable method for simulating complex ground water flow processes in coastal environments and can be used to quantify rates of submarine ground water discharge. The modeling approach presented in this paper also could be used to evaluate and help manage salt water intrusion in shallow coastal aquifers.

Results from the three-dimensional, variable density ground water flow model suggest that ground water discharges directly to Biscayne Bay and to the tidal portions of the coastal canals. From January 1989 to September 1998,



Figure 9. Boundary conditions and input parameters used for sensitivity analysis of fresh submarine ground water discharge to horizontal grid spacing.

the average rate of simulated fresh ground water discharge directly to the Biscayne Bay coastline was 3.7×10^5 m³/day, which is ~10% of the measured surface water discharge to Biscayne Bay for the same period. For the dry seasons of 1989, 1990, and 1991, model results suggest that fresh ground water discharge exceeded the surface water discharge to Biscayne Bay. During wet seasons, however, fresh ground water discharge is about one order of magnitude less than the surface water discharge. Model results also indicate that most of the submarine ground water discharge rates is due to the low land surface elevations adjacent to Biscayne Bay in the southern area.

The combined rate of simulated fresh ground water discharge to the tidal portions of the Miami, Coral Gables, and Snapper Creek Canals is about $3.3 \times 10^5 \text{ m}^3/\text{day}$, similar to the rate of discharge directly to Biscayne Bay. This suggests that tidal canals are focal points for ground water discharge, intercepting fresh ground water that would have discharged directly to Biscayne Bay. Langevin et al. (1998) observed a similar effect in the Florida Keys, where ground water discharge to tidal canals was as much as 15% of the total fresh water recharge. Field observations suggest that Biscayne Bay has changed from a system controlled by widespread and continuous submarine discharge and overland sheetflow to one controlled by episodic releases of surface water at the mouths of canals. The sole explanation for this change has always been that canals lowered the water table, and thus, submarine ground water discharge has decreased. Results from the numerical model, however, suggest that the interception ability of tidal canals is also an explanation for the decrease in submarine ground water discharge directly to Biscayne Bay and the redistribution of discharge to point locations.

Estimated rates of fresh submarine ground water discharge are sensitive to the treatment of Biscayne Bay as a boundary condition. Stage variations in Biscayne Bay relative to water table fluctuations are significant over tidal, daily, and monthly time scales. Model results suggest that the average monthly stage in Biscayne Bay, which is highest during the wet season and lowest during the dry season, tends to dampen the seasonal signature of submarine ground water discharge. Mathematical representation of Biscayne Bay as a solute-transport boundary also has an effect on simulated rates of fresh ground water discharge. Simulated rates of fresh submarine ground water discharge are less when the bay is treated as a constant concentration boundary than when the bay is treated with a mixed boundary. Without sufficient data on dispersion at the boundary between the aquifer and the bay, a case could be made for using either type of solute transport boundary condition. Further research into this problem may help determine the most defensible approach.

Results from the regional model presented in this paper contain a high level of uncertainty. While the model seems adequately calibrated to heads and canal fluxes, there was no way to calibrate to submarine ground water discharge. This is particularly troublesome considering that the simulated estimate of submarine ground water discharge is only ~2% of the annual rainfall total. The reliability of the simulated submarine ground water discharge estimates will improve as estimates of recharge, surface water and ground water interactions, and evapotranspiration improve. Perhaps the next step is to perform formalized sensitivity analysis and parameter estimation to determine the most sensitive parameters for representing submarine discharge and to quantify confidence intervals for discharge estimates.

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