Approximating the Effects of the Saltwater-Freshwater Interface in a Three-Dimensional Groundwater Flow Model

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Abstract Numerical experiments were performed to investigate how the saltwater freshwater interface could be approximated in a three dimensional groundwater flow model to yield accurate values for hydraulic heads in the freshwater part of a coastal aquifer. These experiments consisted of obtaining solutions for a three dimensional model that represents a coastal aquifer using the groundwater flow code MODFLOW and comparing the results to a three dimensional solution for equivalent freshwater heads using the variable density flow and transport code SEAWAT, which was considered to be the accurate solution to the problem. In the SEAWAT solution (solution one), the seacoast was simulated by specifying a concentration boundary condition with a total dissolved solids (TDS) concentration equal to the TDS of seawater, and the upstream freshwater boundary was represented by a specified flux boundary condition. The MODFLOW solutions (solutions two nine) consisted of solution two: specifying the head at the coastal boundary equal to the seawater potential (h_{sw} = 0); solution three: specifying the head at the coastal boundary equal to the equivalent freshwater head (h_{fw}); solution four: using inactive cells to represent the saltwater freshwater interface and specifying the head at the coastal boundary equal to the seawater potential (hsw = 0); solution five: using inactive cells to represent the saltwater freshwater interface and specifying the head at the coastal boundary equal to the equivalent freshwater head (h_{fw}); solution six: reducing the horizontal hydraulic conductivity in model cells to account for reduced freshwater thickness in the part of the aquifer in which saltwater intruded beneath the interface and specifying the head at the coastal boundary equal to the seawater potential (hsw = 0); solution seven: reducing the horizontal hydraulic conductivity in model cells to account for reduced freshwater thickness in the part of the aquifer in which saltwater intruded beneath the interface and specifying the head at the coastal boundary equal to the equivalent freshwater head (h_{fw}); solution eight: designating general head boundary cells along the location of the saltwater freshwater interface and specifying the head at the coastal boundary equal to the seawater potential (h_{sw} = 0); and solution nine: designating general head boundary cells along the location of the saltwater freshwater interface and specifying the head at the coastal boundary equal to the equivalent freshwater head (h_{fw}). The three dimensional MODFLOW solution that best matches the SEAWAT solution in terms of the calculated head at the upstream specified flux boundary is solution three, in which the head at the coastal boundary is specified equal to the equivalent freshwater head (h_{fw}) over the full thickness of the aquifer at the seacoast.

Index Terms **coastal aquifers, hydraulic heads, MODFLOW, numerical experiments, numerical modeling, saltwater freshwater interface, SEAWAT.**

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I. INTRODUCTION

In regional groundwater flow models that border the seacoast, the saltwater-freshwater interface at the seacoast is represented by various approximations. In some models, for example, it is assumed that the saltwater-freshwater interface is stable and flowing freshwater occurs above the interface and static saltwater exists beneath the interface. In these models, inactive cells are used to represent the saltwater part of the aquifer and a no-flow boundary along the interface. In other applications, the coastal boundary is specified as a head-dependent flux boundary condition, and values for the specified heads are equal to the seawater potential or to equivalent freshwater heads. In addition, sharp-interface models and variable-density groundwater flow and transport models also are used to simulate saltwater and freshwater in coastal aquifers. The objective of the investigation described in this paper was to determine how the saltwater-freshwater interface could best be represented in groundwater flow models using a code such as MODFLOW (McDonald and Harbaugh, 1988). Numerical experiments were performed to investigate how the presence of a saltwater-freshwater interface should be approximated in a groundwater flow model to yield accurate values for hydraulic heads in the freshwater part of a coastal aquifer.

A. *Selection of Variable Density Code:*

SEAWAT (Langevin, 2001; Guo and Langevin, 2002), which simulates three-dimensional, variable-density groundwater flow following a modular structure similar to MODFLOW, was used to represent the saltwater-freshwater interface. In SEAWAT, the dependent variable is the equivalent freshwater head:

$$h_{fw} = \frac{P_N}{\rho_f g} + Z_N \qquad (1)$$

where h_{fw} is equivalent freshwater head; P_N is pressure at point N; ρ_f is density of freshwater; g is acceleration due to gravity; and Z_N is the elevation of point N above a datum. The equivalent freshwater head and the head in a saline aquifer are related by:

$$h_{fw} = \frac{\rho}{\rho_f} h - \frac{\rho - \rho_f}{\rho_f} Z \qquad (2)$$

where h is hydraulic head; and ρ is density of saline groundwater at point N.

B. Design of Numerical Experiments:

The numerical experiments consisted of obtaining solutions with different approximations and boundary conditions using MODFLOW and comparing the results to a solution obtained using SEAWAT. A three-dimensional model that consisted of 31 rows, 50 columns, and 40 layers was used to represent a coastal aquifer. The rows were equally spaced with $\Delta y = 250$ m for a total width of 7,750 m, the columns were equally spaced with $\Delta x = 250$ m for a total length of 12,500 m, and the layers were equally spaced with $\Delta z = 5$ m for a total depth of 200 m (see Figure 1). The upstream boundary condition was a specified-flux boundary condition with a flux of 2.0 m2/day, and the coastal boundary condition was a specified-head boundary condition. The concentration at the coastal boundary was specified as constant and equal to 35 kg/m3, representing the total dissolved solids (TDS) concentration of seawater. In the SEAWAT solution, equivalent freshwater heads at the coastal boundary were calculated over the vertical using Equation 2 with h = 0, ρ = 1025 kg/m3, and ρf = 1000 kg/m3. The dimensions of the model, the boundary conditions at the seacoast, the hydraulic conductivities, dispersivities, and other aquifer parameters were chosen so that the model was representative of a field-scale coastal aquifer such as the Floridan aquifer system in the southeastern U.S.A. (see Table 1)

TABLE 1. AQUIFER PARAMETERS AND BOUNDARY INFLOW USED IN NUMERICAL EXPERIMENTS

Parameter	Value
Horizontal hydraulic conductivity (K_H)	50 m/day
Vertical hydraulic conductivity (K_V)	0.5 m/day
Longitudinal dispersivity (α_H)	125 m
Transverse dispersivity (α_T)	12.5
Vertical dispersivity (α_V)	1.25 m
Porosity (η)	0.30
Flow per unit width (Q/W)	2.0 m^2/day

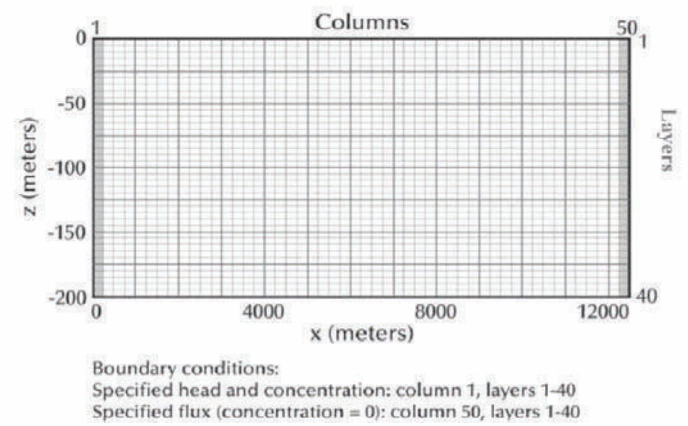

Fig.1. Finite-difference grid used for numerical experiments.

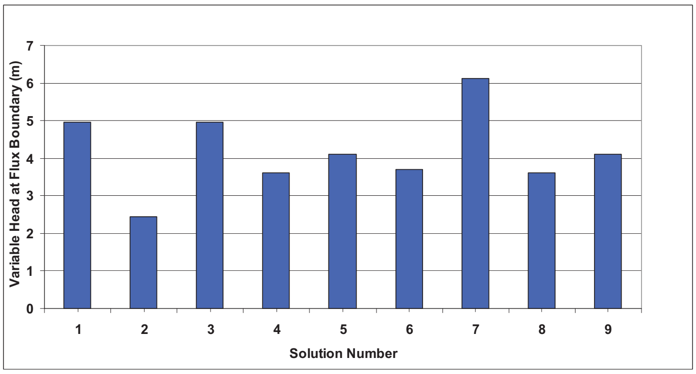

Fig 2. Comparison of solutions for three-dimensional model with specified-flux boundary condition

C. SEAWAT and MODFLOW Solutions:

Nine solutions were calculated using SEAWAT and MODFLOW. For solution one, TDS concentrations and equivalent freshwater heads were calculated using SEAWAT, which was considered to be the accurate solution to the problem. Hydraulic heads also were calculated using MODFLOW to obtain eight additional solutions:

- solution two: the head at the coastal boundary was specified equal to the seawater potential (hsw = 0);
- solution three: the head at the coastal boundary was specified equal to the equivalent freshwater head (hfw), which increased with depth based on Equation 2;
- solution four: inactive cells were used to represent the saltwater-freshwater interface (based on solution one), and the head at the coastal boundary was specified equal to the seawater potential (hsw = 0);
- solution five: inactive cells were used to represent the saltwater-freshwater interface (based on solution one), and the head at the coastal boundary was specified equal to the equivalent freshwater head (hfw), which increased with depth based on Equation 2;
- solution six: the horizontal hydraulic conductivity was

reduced in model cells to account for reduced freshwater thickness in the part of the aquifer in which saltwater intruded beneath the interface (based on solution one), and the head at the coastal boundary was specified equal to the seawater potential (hsw = 0);

• solution seven: the horizontal hydraulic conductivity was reduced in model cells to account for reduced freshwater thickness in the part of the aquifer in which saltwater intruded beneath the interface (based on solution one), and the head at the coastal boundary was specified equal to the equivalent freshwater head (hfw), which increased with depth based on Equation 2;

• solution eight: thirty-two general-head boundary cells were designated along the location of the saltwater-freshwater interface (based on solution one), and the head at the coastal boundary was specified equal to the seawater potential (hsw = 0); and

• solution nine: thirty-two general-head boundary cells were designated along the location of the saltwater-freshwater interface (based on solution one), and the head at the coastal boundary was specified equal to the equivalent freshwater head (hfw), which increased with depth based on Equation 2.

D. Results of Numerical Experiments:

The investigation described in this paper focused on how the presence of the saltwater-freshwater interface could be approximated using MODFLOW to yield accurate values for hydraulic heads in the freshwater part of a coastal aquifer. Accordingly, the heads at the upstream freshwater boundary in the eight MODFLOW solutions were tabulated and compared to the corresponding equivalent freshwater head at the upstream boundary in the SEAWAT solution (see Table 2). Freshwater occurred at this location in the SEAWAT solution, and thus the hydraulic heads calculated in the MODFLOW solutions could be compared directly to the equivalent fresh¬water head in the SEAWAT solution. The three-dimensional MODFLOW solution that best matches the SEAWAT solution in terms of the calculated head at the upstream specified-flux boundary is solution three, i.e., specifying equivalent freshwater heads (hfw) at the coastal boundary over the full thickness of the aquifer at the seacoast (Table 2).

Discussion: The results presented in this paper are supported by the results from other numerical experiements (Motz and Sedighi, 2004), in which the effects of specified-flux and specified-head boundary conditions at the upstream freshwater boundary are tested for both two-dimensional and three-dimensional models. In these results, the MODFLOW solution in which equivalent freshwater heads are specified at the coastal boundary over the full thickness of the aquifer consistently matches the SEAWAT results at the upstream boundary. The results from this investigation are for a field-scale regional aquifer, which complements and expands results such as those reported by Simpson and Clement (2003, 2004) for the smaller-scale Henry and Elder problems.

Table 2. Comparison of solutions for three-dimensional model with specified-flux boundary condition

Solution Number	Variable Head at Specified-Flux Boundary (m)
SEAWAT Solution:	
1	4.95
MODFLOW Solutions:	
2	2.45
3	4.95
4	3.61
5	4.11
6	3.70
7	6.13
8	3.62
9	4.11

II. CONCLUSIONS:

Based on the results of the numerical experiments described in this paper, the effects of the saltwater-freshwater interface can be represented in a three-dimensional MODFLOW simulation by specifying equivalent freshwater heads at the coastal boundary over the full thickness of the aquifer, which is represented by solution three in this investigation. These results could be used to evaluate whether existing regional models have correctly represented the effects of the saltwater-freshwater interface, which would affect the accuracy of hydraulic heads predicted in the freshwater part of the aquifer near the interface. Also, these results could be used as a guide during the construction of new regional groundwater flow models to ensure that heads in the freshwater part of the aquifer will be calculated correctly.

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