MODSHARP: Regional-Scale Numerical Model for Quantifying Groundwater Flux and Contaminant Discharge into the Coastal Zone

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ABSTRACT


The groundwater flux to coastal water can be a major component of the water balance in coastal zone. In this paper we report the developing of a quasi-three-dimensional numerical model that can be used for quantifying groundwater inputs and associated contaminant discharged from coastal aquifers into the coastal zone at regional-scale. The present model is called MODSHARP. Sharp interface approach for conceptualisation of seawater intrusion is applied in this model in order to be able to handle problems in regional-scale. Method of characteristics is used to solve advection-dispersion equation, governing to contaminant transport in the coastal aquifer. The model can be used for simulation of groundwater flow and contaminant transport in layered coastal aquifer at regional-scale. The present regional-scale numerical model can be used to develop a better understanding of the interactions between water bodies in coastal zone. It can also be used to predict the fate of contaminant plume in coastal aquifers and therefore allow for better strategies to be implemented to control or mitigate the effects of contaminants on coastal wetlands, coastal aquifers, and the adjacent marine environment.

ADITIONAL INDEX WORDS: Coastal aquifers, ocean-land interface, saltwater intrusion, numerical simulation.

INTRODUCTION

It is necessary to have a proper estimate of the groundwater inputs to coastal waters for a successful integrated coastal zone management. The groundwater flux to coastal water can be a major component of the water balance in coastal zone. In some cases it is as high as 40% of riverwater flux into coastal water (MOORE 1996). Moreover, the contaminants and nutrients are carried by groundwater flow and discharged into coastal water have a considerable influence on environmental management of coastal zone.

Until recently, the principal concern associated with the hydrological connection between groundwater and the ocean has been that associated with saline water intrusion into coastal water supplies. Increasingly, however, there is concern that submarine and marginal marine discharges of nutrient- and contaminant-rich groundwater may have a more significant impact on material fluxes than implied by the relative magnitudes of groundwater and surface water discharges. Seep zones in many settings appear to be associated with unique and important marginal marine and inter-tidal biological communities of high productivity. Therefore, these discharges may also play an important role in local biodiversity, in ecosystem function, and potentially in contaminant transfer up the marine and terrestrial food chains (ULLMANN, et al., 2003).

Numerical model can be utilized to simulate the groundwater flow and contaminant transport in coastal aquifers. However, there are serious limitations in the available numerical models for application at regional-scale.

ATAIE-ASHTIANI et al. (1999a and 1999b) presented a numerical model for simulation of groundwater flow in coastal aquifers that could handle tidal fluctuations and seepage-face condition at the seaward boundary. In their model the seawater intrusion into the coastal aquifer were simulated using dispersed interface approach. However, the model can be used either for simulation of contaminant transport or the seawater intrusion. Besides, solving density-dependent flow for depressive interface approach is computationally demanding and therefore it imposes sever limitations on the scale of considered aquifer for simulation.

In this paper the developing of a quasi-three-dimensional numerical model that can be used for quantifying groundwater inputs and associated contaminant discharged from coastal aquifers into the coastal zone at regional-scale is reported. The present model is called MODSHARP. The salt-water intrusion phenomenon in groundwater systems has been conceptualised by two general approaches: the sharp interface approach and the dispersed interface approach. In the former it is assumed that the salt-water and freshwater are immiscible fluids separated by a sharp interface. In the latter a transition zone of mixed salt and fresh water is considered to be present at the interface. Sharp interface approach is computationally less demanding in comparison to dispersed interface approach. Sharp interface approach is applied in this model in order to be able to handle problems in regional-scale.

Method of characteristics is used to solve advection-dispersion equation, governing to contaminant transport in the coastal aquifer. The model can be used for simulation of groundwater flow and contaminant transport in layered coastal aquifer at regional-scale. The mathematical formulation and numerical methods are presented in next section. The numerical model results are successfully verified by comparison with some of the available semi-analytical solutions and also experimental data.

MATHEMATICAL AND NUMERICAL MODELS

In this study SHARP Model (ESSAID, 1989) has been improved and modified for modelling the groundwater flow and contaminant transport in coastal aquifers. SHARP is a quasi-three-dimensional, finite difference model that simulates fresh water and salt water flow separated by sharp interface in layered coastal aquifer systems. Vertically integrated fresh water and salt water flow equations, incorporating the interface boundary condition and leakage terms calculated by Darcy's law, are solved within each aquifer. The governing equations describing the SHARP fluid mass balance are (ESSAID, 1989):
where \( \Phi_f \) and \( \Phi_s \) are fresh and salt water hydraulic conductivities in x-direction \([LT^{-1}]\), \( K_f \) and \( K_s \) are fresh and salt water hydraulic conductivities in y-direction \([LT^{-1}]\), \( B_f \) and \( B_s \) are fresh and salt water specific weights \([MLT^{-2}]\), \( \alpha \) is 1 for an unconfined aquifer and 0 for a confined aquifer. This system of coupled non linear partial differential equations for contaminant transport is discretized using an implicit finite difference scheme that is central in space and backward in time. The locations of the interface tip and toe within grid blocks are tracked by linearly extrapolating the position of the interface based on the known grid point elevations. The discretized form of equations is solved using the strongly implicit procedure SIP for three dimensional two phase flow.

In the present work the equation of two-dimensional areal contaminant transport is solved using an implicit finite difference scheme that is central in space and backward in time. The locations of the interface tip and toe within grid blocks are tracked by linearly extrapolating the position of the interface based on the known grid point elevations. The discretized form of equations is solved using the strongly implicit procedure SIP for three dimensional two phase flow.

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The method of characteristics (MOC) is used in MODSHARP model to solve the solute-transport equation. The method has been successfully applied to variety of field problems of flow (Konikow and Bredehoeft, 1978). The approach taken by MOC is not to solve equation (3) directly, but rather to solve an equivalent system of ordinary differential equations.

The first step in the MOC involves placing a number of traceable particles in each cell of finite difference grid to form a set of points that are distributed in a geometrically uniform pattern throughout the area of interest. It was found that placing four to nine points per cell provided satisfactory results for most two-dimensional problems. The initial concentration assigned to each point is the initial concentration associated with the node of the cell containing the point (Konikow and Bredehoeft, 1978).

For each time step every point is moved a distance proportional to the length of the time increment and the velocity at the location of the point. After all points have been moved, the concentration at each node is temporarily assigned the average of concentrations of points that located within the area of that cell. The moving points simulate convective transport because the concentration at each node of the grid will change with each time step as different points having different concentrations enter and leave the area of that cell. The changes in concentration caused by hydrodynamic dispersion, fluid sources, divergence of velocity, and changes in saturated thickness are calculated using an explicit finite-difference approximation.

**EVALUATION OF MODSHARP**

The accuracy of numerical solution to the solute transport equation that has been added to SHARP model can be evaluated in part by analyzing relatively simple problems for which analytical solutions are available and than comparing the numerical calculations with the analytical solution. A series of this type of test has been performed to check the MODSHARP model. The results of one of these cases are presented in this section. Unfortunately there is no analytical solution for the cases that the saltwater intrusion into the coastal aquifer is occurred all together with transport of contamination in the aquifer. An example for this case is also presented in this section to show the capability of MODSHARP in simulation of contaminant transport in coastal aquifer exposed to saltwater intrusion.

**Case 1 Simulation of Contaminant Transport by of Pulse Source.**

If a pulse of contaminant is injected over the full thickness of a two-dimensional homogeneous aquifer, it will move in the direction of flow and spread out with time. If a tracer with concentration \( C \) is injected over an area \( A \) at a point \((x_c, y_c)\), the concentration at any point \((x, y)\) at time \( t \) after the injection is given by the following equation (De Josselin De Jong, 1958).

\[
\int_0^t \left( \frac{Q}{n} \right)_{i,j} \ dC = V \left( \frac{C}{n} \right)_{i,j} - \frac{C}{n} \left( \frac{Q}{n} \right)_{i,j} \]

where \( C \) is the concentration of the dissolved chemical species \([ML^{-1}]\), \( V \) is the seepage velocity in the direction of \( x \) \([LT^{-1}]\), \( D \) is the coefficient of hydrodynamic dispersion \([LT^{-2}]\), \( B \) is the saturated thickness of the aquifer \([L]\), \( n \) is the effective porosity of the aquifer \([-]\), \( B \) is the volume flux per unit area \([LT^{-1}]\), and \( C' \) is the concentration of dissolved chemical in a source or sink fluid \([ML^{-1}]\). The seepage velocity is determined from Darcy’s law:

\[
V = \frac{K}{n} \frac{\partial \Phi}{\partial x} \]

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Figure 2. (a) Schematic of considered coastal aquifer, (b) Concentration contours of 10, 50 and 90 percent after 100 years, (c) Concentration contours of 10, 50 and 90 percent of C after 200 years, and (d) Location of saltwater and fresh water interface.
of 10 km and thickness of 204 m is considered. A schematic of aquifer is shown in Figure 2.a. The horizontal and vertical hydraulic conductivity of aquifer are 100 m/day and 10 m/day, respectively, the porosity is 0.4, and the fresh and saltwater specific storages are 10$^{-7}$ and 1.03x10$^{-6}$ m$^{-3}$, respectively. A constant head of 24.1 m at landside and 0.072 m at sea side are considered that cause a constant hydraulic gradient of 0.0012 toward sea. The fresh and saltwater densities are 1000 kg/m$^3$ and 1030 kg/m$^3$. A contamination source with constant concentration of 1 mg/l, $C_s$, in an area of 2000x500 m in the middle of land ward boundary is considered. The longitudinal and transverse dispersions of $D_L=100$ m and $D_T=20$ m are assumed (where $D_L=\alpha_L|V|$ and $D_T=\alpha_T|V|$). For numerical simulation blocks of 500x500 m are considered. Therefore the number of blocks is 840 (20x24) and time step is 1 day.

Figure 2.b and 2.c illustrate the concentration contours of 10, 50 and 90 percent of $C_s$ after 100 years and 200 years. Also the location of salt and fresh water interface is shown in Figure 2.d. The results show a reasonable distribution for contaminant and also interface position. As seen, MODSHARP has the capability of simulation of groundwater flow and contaminant transport in coastal aquifer at regional-scale.

CONCLUSIONS

The seaward boundary of coastal aquifers has significant influence on the groundwater flow and the amount of contaminant discharged from coastal aquifers into the coastal waters. A regional-scale numerical (MODSHARP) was developed and tested in this work. The present numerical model can be used to develop a better understanding of the interactions between water bodies in coastal zone. It can also be used to predict the fate of contaminant plume in coastal aquifers and therefore allow for better strategies to be implemented to control or mitigate the effects of contaminants on coastal wetlands, coastal aquifers, and the adjacent marine environment.

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LITERATURE CITED


