United States Environmental Protection Agency

€PA

National Risk Management Research Laboratory Ada, OK 74820

EPA/600/SR-99/110

January 2000

Research and Development

Project Summary

Analytic Element Modeling of Coastal Aquifers

Mark Bakker, Stephen R. Kraemer, Willem J. de Lange, and Otto D.L. Strack

Four topics were studied concerning the modeling of groundwater flow in coastal aquifers with analytic elements: (1) practical experience was obtained by constructing a groundwater model of the shallow aquifers below the Delmarva Peninsula USA using the commercial program MVAEM; (2) a significant increase in performance was obtained by implementing the theory for variable density flow in a computer program that ran on a supercomputer using vectorization; (3) a new representation for the density variation was developed that can simulate the change from brackish to fresh water more accurately; and (4) it was shown that for a specific example of a bellshaped transition zone a Dupuit model gives accurate results unless the bellshape is too narrow compared to the thickness of the aquifer.

This Project Summary was developed by EPA's National Risk Management Research Laboratory's Subsurface Protection and Remediation Division, Ada, OK, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Salt water intrusion is a potential threat to drinking water supplies in the coastal areas of the USA. Cities along the coast are increasing their pumping of groundwater, which may result in an increase of chlorides in the well water due to the upconing of brackish groundwater. Even a small concentration of chlorides (> 0.2 grams/liter) will violate the drinking water standard. To compare, sea water contains about 18 grams of chlorides per liter. The potential upconing of brackish groundwater may be studied by the simulation of groundwater flow with numerical models that are designed specifically for the modeling of flow in coastal aquifers.

Groundwater flow in coastal aquifers is affected by the difference in density between fresh and salt water. The fresh water is separated from the salt water through a brackish transition zone, in which the salinity (and thus the density) of the water varies from that of salt water to that of fresh water; salt water is approximately 2.5% heavier than fresh water. The modeling of the flow generated by variations in density, the variable density flow, was the subject of this project. Specifically, it was investigated whether groundwater flow in coastal aquifers can be modeled under the Dupuit approximation in combination with analytic elements.

The Dupuit Approximation

The construction of numerical models of three-dimensional variable density flow is limited by the availability of density data and by the speed of digital computers. The Dupuit approximation may be adopted to reduce the computation time and for the usual reason of simplicity. The resistance to flow in the vertical direction is neglected in Dupuit models, and vertical flow is governed by continuity of flow only; this leads to a hydrostatic pressure distribution in the vertical direction. The Dupuit approximation is reasonable for flow in aquifers of large horizontal extend, also referred to as aquifers with shallow flow or regional flow. It is possible to construct regional groundwater flow models of coastal aquifers by adopting the Dupuit approximation. The Dupuit theory for variable density flow may be combined with any method to model Dupuit flow in a single density model. The flow field is modeled with analytic elements for this project.

The Dupuit theory for variable density flow assumes that the density distribution in the aquifer is known at some time. In practice, the density is known only at a number of isolated points. We represent the density distribution with a threedimensional function that interpolates between the points of known density. We use the multiquadric radial basis interpolator for this purpose. It is noted that the multiquadric interpolator is a form of Kriging; the interpolator is identical to Kriging with a linear variogram if the shape factor in the interpolator is set equal to zero.

The density distribution (and thus the flow field) changes over time as the salt moves with the groundwater flow. The flow is incompressible in our model and the flow field represents the flow at a given time. The evolution of the density distribution in the aquifer may be simulated by numerical integration through time. During each time step, the velocity field is fixed and the salt is moved with the groundwater flow. At the end of a time step the velocity field corresponding to the new density distribution is computed and the process is repeated. This procedure is also known as successive steady-state solutions. Second order processes that affect the salinity distribution, such as diffusion, are neglected. It may be expected that this is reasonable for relatively short times, on the order of 25 years, as is of interest for most engineering problems.

The Dupuit theory for variable density has been implemented in the proprietary computer program MVAEM prior to this study. MVAEM has been used successfully to simulate piezometric heads in multiaquifer systems in the coastal aquifers of The Netherlands. The computation time involved in the construction of these large regional models was significant. Multi-layer models that include thousands of points where the salinity is specified take on the order of hours to compute a solution on a high end PC (in 1996). A large portion of the computation time is used to compute the effect of the variation in density on the flow. The computation times of the transient simulations involve a repeated computation of the solution at different times plus a large number of evaluations of the velocity in the aquifer and is of the order of days or more, as compared to the hours it takes to obtain one steady-state solution. These large computation times diminish the practicality of the modeling approach.

The use of a Dupuit model to simulate variable density flow raises a number of additional issues. Transient simulations require an accurate representation of the velocity field and the numerical integration requires an analysis of stability and convergence. Furthermore, it must be investigated how accurate a Dupuit model is to simulate the change of a salt distribution over time as compared to a model in which the vertical resistance to flow is not neglected. Dupuit models are generally used for regional (shallow) flow and may become inaccurate when the shallow flow assumption is not appropriate, for example near a partially penetrating well where the flow field changes rapidly over a distance of several times the aquifer thickness. And finally, the assessment of the upconing of salt water below a pumping well needs analysis of the physical stability of the transition zone itself. A selection of the issues raised above has been investigated in this project.

Objectives

The objective of this report is to investigate the performance of the Dupuit theory for variable density flow combined with analytic elements to model groundwater flow in coastal aquifers. The four specific areas of interest are (1) the application of a Dupuit analytic element model to simulate flow in a coastal aquifer of the USA, (2) the increase in performance that may be obtained by using a supercomputer, (3) the representation of the density distribution, and (4) the error introduced by adopting the Dupuit approximation.

Results and Conclusions

Topic 1. The analytic element modeling of groundwater flow in the first confined aquifer beneath the Delmarva Peninsula.

An analytic element model was constructed to simulate ground-water flow in the shallow aquifers beneath the Delmarva Peninsula (DELaware, MARyland, VirginiA). The modeling of the Delmarva peninsula was greatly hampered by the unavailability of measurements of the salinity of the groundwater. Only six measurements were obtained (from available records) of brackish or salt water. All other measurements indicated fresh water. The six measurements were insufficient to construct a three-dimensional picture of the salinity distribution below the Delmarva Peninsula. To overcome this problem, publications of salinity in the Chesapeake Bay and the Atlantic Ocean were used to construct a conceptual model of the salinity distribution below the peninsula. This distribution results in a horizontal variation from fresh water on the peninsula to salt water in the bay and ocean. The variation in the vertical direction is assumed to be negligible. This is known to be unrealistic, but there are not enough data to propose otherwise.

The resulting model of the fresh water head was compared to nine measurements of the head on the eastern part of the peninsula (the counties of Sussex, DE, Wicomico, MD, and Worchester, MD). The comparison showed that the simulation of fresh water heads in that area are reasonable, but general conclusions for the entire model cannot be drawn. Additional data (head, discharge and chloride measurements) are necessary to calibrate the model and to improve the conceptual model of the density distribution. The modeling study demonstrated the many challenges in building groundwater models of flow systems in coastal aquifers. The biggest constraints in the Chesapeake Bay area were the availability of density data and water table measurements. To assess the full capabilities of the approach, it should be applied to an area where more data are available, perhaps an area outside the United States.

Topic 2. The reduction of computation time by the use of a supercomputer.

The Dupuit approximation for variable density flow was implemented in an existing analytic element model (SLWL) that was written in FORTRAN. The variable density routines were written to run on the CrayC916, a vector machine. The Dupuit formulation for variable density flow, as well as the analytic element formulation for groundwater flow, are suited ideally for implementation on supercomputers. Both formulations result in large sums of complicated functions that are easily vectorizable. The performance of the vectorized code was an order of magnitude better than the un-vectorized code. The vectorized code performed at a speed of over 300 billion floating point operations per second (300 Gflops).

It is noted that high performance computing seems to move away from vector machines to massively parallel machines. This will have no adverse effect on the implementation of analytic element codes on supercomputers. The large sums of complicated functions can just as easily be modified to run on massively parallel machines as on vector machines.

Topic 3. An accurate representation of the density distribution.

For the investigation of the first two topics, the density distribution was represented by the three-dimensional multiquadric interpolator function. The multiquadric interpolator includes a shape factor Δ that controls the smoothness of the interpolator. In practice, Δ is often chosen close to zero. The main reason for this choice is to improve control of the interpolator, especially at the transition from brackish water of variable density to fresh or salt water of constant density. It was demonstrated that this choice will result in reasonable simulations of the density (and thus the fresh water head, as was the objective of the modeling study of the Delmarva Peninsula), but that the resulting velocity vector was unrealistic near the points where the density is specified. This makes it difficult to simulate the change of the salinity distribution through time; during such a simulation the salt moves with the groundwater and the velocities have to be accurate.

A new function to represent the density was introduced to solve this problem. The representation consists of a number of surfaces of constant density; the elevations of the surfaces are approximated with two-dimensional multiquadric interpolators and the density varies linearly between them. It was shown that the smoothness parameter Δ in the two-dimensional multiquadric interpolator must be of the order of the average distance between control points to obtain reasonable results for the velocity field. It is noted that this was not practical for the original three-dimensional interpolator.

Topic 4. Implications of adopting the Dupuit approximation for variable density flow.

The new density distribution was used to compare a Dupuit solution with an exact solution, a solution in which the vertical resistance to flow is not neglected. The problem chosen for comparison consisted of a bell-shaped transition zone. An exact solution was derived and compared to the Dupuit solution. The comparison showed that for this specific case the Dupuit solution overestimates the specific discharge vector and that the flow field becomes inaccurate when the width of the bell-shaped transition zone is less than two times the thickness of the aquifer.

The new density distribution, as proposed under "Topic 3," represents the transition from variable density zones (brackish water) to constant density zones (fresh or salt water) accurately. The new distribution does introduce complications that remain to be resolved, however, such as the intersection of the transition zone with the base or top of the aguifer. The new density distribution is highly useful for the comparison of Dupuit solutions with exact solutions, because it is relatively easy to obtain exact solutions for flow in the vertical plane corresponding to the new density distribution. A comparison between exact and Dupuit solutions may be used to determine the full range of applicability of the Dupuit approximation for variable density flow.

Mark Bakker was with the University of Minnesota during this project but is currently with the University of Nebraska, Omaha, NE 68182. Willem J. de Lange is with the National Institute of Inland Water Management RIZA, Lelystad, The Netherlands. Otto D.L. Strack is with the University of Minnesota, Minneapolis, MN 55455. Stephen R. Kraemer was the EPA Project Officer while at the EPA National Risk Management Research Laboratory in Ada, OK 74820, and is currently at the EPA National Exposure Research Laboratory in Athens, GA 30605. The complete report, entitled "Analytic Element Modeling of Coastal Aquifers" (Order No. PB2000-101970: Cost: \$29.50, subject to change) will be available from: National Technical Information Service 5285 Port Royal Road Springfield, VA 22161 Telephone: 703-487-4650 An electronic version of this Project Summary and the Full Report will be available for download on the Internet at (http://www.epa.gov/ada/kerrcenter.html)

United States Environmental Protection Agency Technology Transfer and Support Division (CERI) Cincinnati, OH 45268

Official Business Penalty for Private Use \$300

EPA/600/SR-99/110

BULK RATE POSTAGE & FEES PAID EPA PERMIT No. G-35