Coastal Aquifer Management

Monitoring, Modeling, and Case Studies

Alexander H.-D. Cheng
Driss Ouazar

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CHAPTER 3

MODFLOW-Based Tools for Simulation of Variable-Density Groundwater Flow

Christian Langevin, Gualbert Oude Essink, Sorab Panday, Mark Bakker, Henning Prommer, Eric Swain, Walter Jones, Michael Beach, Mark Barcelo

1. INTRODUCTION

Most scientists and engineers refer to MODFLOW [McDonald and Harbaugh, 1988; Harbaugh and McDonald, 1996; Harbaugh et al., 2000] as the computer program is the most widely used program for constant-density groundwater flow problems. [GOE: why double space after every sentence?] The success of MODFLOW is largely attributed to its thorough documentation, modular structure, which makes the program easy to modify and enhance, and the public availability of the source code. MODFLOW has even been referred to as a "community model," because of the large number of packages and utilities developed for the program [Hill et al., 2003]. In recent years, the MODFLOW code has been adapted to simulate variable-density groundwater flow. Because MODFLOW is so widely used, these variable-density versions of the code are rapidly gaining acceptance by the modeling community.

The basic approach for using MODFLOW to represent variable-density groundwater flow is to formulate the flow equation in terms of equivalent freshwater head. With this approach, the finite-difference representation can be rewritten so that fluid density is isolated into mathematical terms that are identical in form to source and sink terms. These "pseudo-sources" can then be easily incorporated into the matrix equations solved by MODFLOW. Weiss [1982] was one of the first to recast the groundwater flow equation in terms of equivalent freshwater head and introduce the concept of a pseudo-source. Lebbe [1983] used a similar approach to develop a variable-density version of the MOC code [Konikow and Bredehoeft, 1978]. Maas and Emke [1988] were among the first to incorporate variable-density flow into MODFLOW. The approach was improved by Olsthoorn [1996] to account for inclined model layers. These initial studies allowed for fluid density to vary in space, but not in time. Recently, solute transport codes have been linked directly with

MODFLOW to represent the transient effects of an advecting and dispersing solute concentration field on variable-density groundwater flow patterns. These MODFLOW-based codes are being applied to numerous hydrologic problems involving variable-density groundwater flow.

Descriptions and applications of four of the commonly used MODFLOW-based computer codes are presented in this chapter. The four codes (SEAWAT, MOCDENS3D, MODHMS, and the Sea Water Intrusion Package for MODFLOW-2000) have been applied to case studies and have been documented and tested with variable-density benchmark problems. The first three programs described in this chapter represent advective and dispersive solute transport. The fourth program uses a semi-analytical non-dispersive approach to simulate movement of multiple density isosurfaces.

2. SEAWAT

Christian Langevin, Henning Prommer, and Eric Swain

The SEAWAT computer program is designed to simulate a wide range of hydrogeologic problems involving variable-density groundwater flow and solute transport. The SEAWAT code has been applied worldwide to evaluate such problems as saltwater intrusion, submarine groundwater discharge, aquifer storage and recovery, brine migration, and coastal wetland hydrology. The source code, documentation, and executable computer program are available to the public from the following web page: http://water.usgs.gov/ogw/seawat/.

This section provides a brief description of the SEAWAT program and presents applications of SEAWAT to geochemical modeling and integrated surface water and groundwater modeling. Additional information, including the SEAWAT documentation, is included on the CD-ROM.

2.1 Program Description

SEAWAT was designed by combining MODFLOW-88 and MT3DMS into a single program that solves the coupled variable-density groundwater flow and solute-transport equations [Guo and Bennett, 1998; Guo and Langevin, 2002]. The flow and transport equations are coupled in two ways. First, the fluid velocities that result from solving the flow equation are used in the advective term of the solute-transport equation. Second, the solute-transport equation is solved, and an equation of state is used to calculate fluid densities from the updated solute concentrations. These fluid densities are then used directly in the next solution to the variable-density groundwater flow equation.

The variable-density groundwater flow equation solved by SEAWAT is formulated using equivalent freshwater head as the principle dependent variable. In this form, the equation is similar to the constant-density groundwater flow equation solved by MODFLOW. Thus, with minor modifications, MODFLOW routines are used to represent variable density groundwater flow. Modifications include conservation of fluid mass, rather than fluid volume, and the addition of relative density difference terms, or pseudo-sources. The procedure for solving the variable-density flow equation is identical to the procedure implemented in MODFLOW. Matrix equations are formulated for each iteration, and a solver approximates the solution. Modifications are not required for the MT3DMS routines that solve the transport equation.

Like MT3DMS, SEAWAT divides simulations into stress periods, flow timesteps, and transport timesteps. The lengths for stress periods and flow timesteps are specified by the user; however, the time lengths for transport timesteps are calculated by the program based on stability criteria for an accurate solution to the transport equation. Because flow and transport are coupled, either explicitly or implicitly, the flow and transport equations are solved for each transport timestep. This requirement does not apply for simulations with standard MODFLOW and MT3DMS because in that case, concentrations do not affect the flow field.

Output from SEAWAT consists of equivalent freshwater heads, cell-by-cell fluid fluxes, solute concentrations, and mass balance information. This output is in standard MODFLOW and MT3DMS format, and most commercially available software can be used to process simulation results. For example, animations of velocity vectors and solute concentrations can be prepared using the U.S. Geological Survey's Model Viewer program [Hsieh and Winston, 2002], and post-processing programs such as MODPATH [Pollock, 1994] can be used to perform particle tracking using SEAWAT output.

The U.S. Geological Survey actively supports the SEAWAT program. As new packages, processes, and utilities are added to the MODFLOW and MT3DMS programs, these improvements are incorporated into SEAWAT. For example, a new version of SEAWAT, which is based on MODFLOW-2000, was recently developed.

2.2 Reactive Transport Modeling with PHREEQC and SEAWAT

Two disciplines namely, reactive transport modeling and variable-density flow modeling, have received significant attention over the past two decades. Well known representatives of the former class of models are, for example, MIN3P [Mayer et al., 2002], GIMRT/CRUNCH [Steefel, 2001], PHREEQC [Parkhurst and Appelo, 1999], PHAST [Parkhurst et al., 1995], TBC [Schäfer et al., 1998]; HydroBioGeoChem [Yeh et al., 1998] and some MODFLOW/MT3DMS-based models such as RT3D [Clement, 1997] and PHT3D [Prommer et al., 2003].

In most cases the separation of the two disciplines is well justified, because (i) density gradients are small enough to be of negligible influence on the reactive transport of multiple solutes or (ii) reactions, in particular water-sediment interactions such as mineral dissolution/precipitation and/or sorption, have a minor effect on the density of the aqueous phase. However, specific cases exist where transport phenomena can only be accurately described by considering simultaneously both variable density and reactive processes. For example, Zhang et al. [1998] were only able to explain the differential downward movement of a lithium (Li^+) and a bromide (Br^-) plume at Cape Cod through multi-species transport simulations that considered the variable density of the plume(s) and lithium sorption. Furthermore, Christensen et al. [2001, 2002] demonstrated the interactions between reactive processes and density variations for a seawater intrusion experiment and for a dense landfill leachate plume.

The ongoing project to combine SEAWAT with the geochemical model PHREEQC-2 was initially motivated by the desire to simulate and quantify reactive changes that occur as a result of tidally induced, variable density flow near the aquifer/ocean interface. Coupling of PHREEQC-2 with SEAWAT is achieved through a sequential operator splitting technique [Yeh and Tripathi, 1989, Barry et al., 2002], similar to the technique used for the PHT3D model, which couples PHREEQC-2 with MT3DMS. The governing equation for both transport and reactions of the i^{th} (mobile) aqueous species/component is:

$$\frac{\partial C_i}{\partial t} = \frac{\partial}{\partial x_\alpha}\left(D_{\alpha\beta} \frac{\partial C_i}{\partial x_\beta} \right) - \frac{\partial}{\partial x_\alpha}\left(v_\alpha C_i \right) + r_{reac,i} , \tag{1}$$

while for immobile entities, such as minerals, the transport terms drop out:

$$\frac{\partial C_i}{\partial t} = r_{reac,i} , \tag{2}$$

where v_α is the pore-water velocity in direction x_α, $D_{\alpha\beta}$ is the hydrodynamic dispersion coefficient tensor, and $r_{reac,i}$ is a source/sink rate due to chemical reaction. C_i is the total aqueous component concentration [Yeh and Tripathi 1989], defined as:

$$C_i = c_i + \sum_{j=1,n_s} Y_j^s s_j , \tag{3}$$

where c_i is the molar concentration of the (uncomplexed) aqueous component, n_s is the number of species in dissolved form that have complexed with the aqueous component, Y_j^s is the stoichiometric coefficient of the aqueous component in the j^{th} complexed species and s_j is the molar concentration of the j^{th} complexed species. Like in PHT3D, the (local) redox-state, pe, is modeled by transporting chemicals/components in different redox states separately, while the pH is modeled from the (local) charge balance.

The splitting scheme used to solve the advection-dispersion-reaction equation (Eq. (1)) for a user-defined time step length consists of two steps. In the first step the advection and dispersion term of mobile chemicals is solved with SEAWAT for the time step length Δt. In the subsequent step the reaction term r_{reac} in Eq. (1) is solved through grid-cell wise batch-type PHREEQC-2 reaction calculations. This step accounts for the concentration changes that have occurred during Δt as a result of reactive processes. The reaction terms r_{reac} in Eq. (1) and Eq. (2) correspond to the concentration differences from before (PHREEQC-2 input concentrations) and after the reaction step (PHREEQC-2 output concentrations).

Fig. 1 illustrates the results from one of the initial (simple) multi-species test simulations of coastal point-source pollution by an organic contaminant. The plume is degraded aerobically, i.e., the degradation reaction creates an oxygen-depleted zone in an aquifer containing groundwater of variable density.

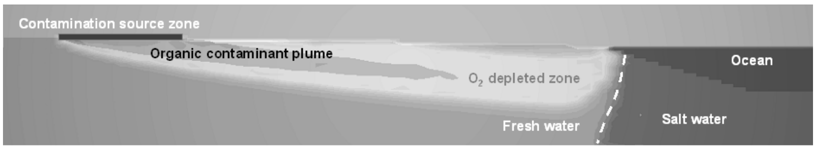


Figure 1: Simulated coastal point source pollution by an aerobically degrading organic contaminant.

2.3 Integrated Surface Water and Groundwater Modeling with SWIFT2D and SEAWAT and Application to the Florida Everglades

2.3.1 Code Description

To simulate the coastal hydrology of the southern Everglades of Florida, which is characterized by shallow overland flow and subsurface groundwater flow, SEAWAT was coupled with the hydrodynamic estuary model, SWIFT2D (Surface-Water Integrated Flow and Transport in 2-Dimensions) [Langevin et. al, 2002; Langevin et al., 2003; Swain et al., 2003]. SWIFT2D solves the full dynamic wave equations, including density effects, and can also represent transport of multiple constituents, such as seawater salts. The SWIFT2D code was originally developed in the Netherlands [Leendertse, 1987], and was later modified by the U.S. Geological Survey to represent overland flow in wetlands by including spatially varying rainfall, evapotranspiration, and wind sheltering coefficients [Swain et al, 2003].

The coupling of SWIFT2D and SEAWAT is accomplished by including the programs as subroutines of a main program called FTLOADDS (Flow and Transport in a Linked Overland-Aquifer Density Dependent System). FTLOADDS uses a mass conservative approach to couple the surface water and groundwater systems, and computes leakage between the wetland and the aquifer using a variable-density form of Darcy’s Law. The leakage representation also includes associated salt transfer, based on leakage rates, flow direction, and salt concentrations in the wetland and aquifer.

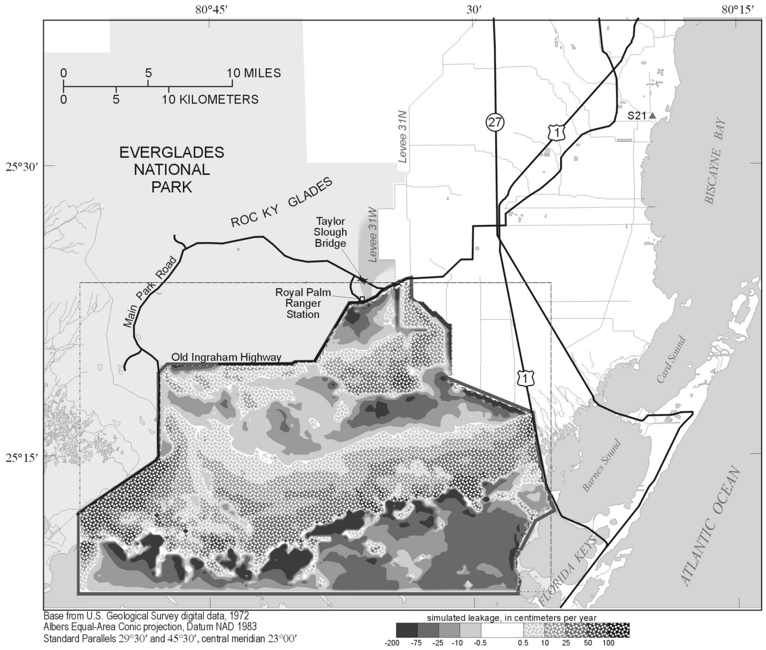
Coupling between SWIFT2D and SEAWAT occurs at intervals equal to the stress period length in the groundwater model. For each stress period, which is one day in the current Everglades application, SWIFT2D is called first, using short timesteps, such as 15 minutes, to complete the entire stress period. Within the SWIFT2D subroutine, leakage is calculated as a function of the surface water stage and the groundwater head from the end of the previous stress period. The total leakage volumes (for each cell) are summed for the stress period by accumulating the product of the leakage rate and the length of the surface water timestep. After SWIFT2D completes the stress period, the total leakage volumes are applied on a cell-by-cell basis to SEAWAT as it runs for the same stress period.

FTLOADDS also accounts for the net salt flux between surface water and groundwater. When the leakage volume is computed for a surface-water timestep, the salt flux is computed based on flow direction. If the flow is upward from the aquifer into the wetland, the salt flux is calculated by multiplying leakage volume and groundwater salinity. The calculated salt mass is then added to the surface-water cell in the SWIFT2D transport subroutine. If flow is downward from the wetland into the aquifer, the salt mass flux is calculated as the product of leakage volume and surface-water salinity. The total salt mass flux is summed for the surface-water timesteps and divided by the total leakage volume. This gives an equivalent salinity concentration for the total leakage over the stress period. Whichever direction of the leakage, the computed equivalent salinity is used in SEAWAT as the concentration of the water added or removed from the aquifer as leakage.

2.3.2 Application to the Southern Everglades of Florida

As part of the Comprehensive Everglades Restoration Plan, the U.S. Geological Survey has applied the FTLOADDS model to the Taylor Slough area in the southern Everglades of Florida (Fig. 2) [Langevin et al. 2002]. The finite-difference grid consists of 148 columns and 98 rows. Each cell is square with 304.8-m per side. The three dimensional grid has 10 layers (each 3.2-m thick) and extends from land surface to a depth of 32 m. The integrated model simulates flow and transport from 1995 through 1999.

The integrated surface water and groundwater model was calibrated by adjusting model input parameters until simulated values of stage, salinity, and flow matched with observed values at the wetland and Florida Bay monitoring sites. Daily leakage rates between surface water and groundwater are produced as part of the model output for each cell. These daily leakage rates were averaged over the 5-year simulation period to illustrate the spatial variability in surface water/groundwater interaction (Fig. 2). These leakage rates do not include recharge or evapotranspiration directly to or from the water table. The model suggests an alternating pattern of downward and upward leakage from north to south (Fig. 2). To the north, most leakage is downward into the aquifer, except near the Royal Palm Ranger station where upward flow occurs near Old Ingraham Highway. Further south, a large area of upward leakage exists. This area of upward leakage roughly corresponds with the position of the freshwater/saltwater transition zone in the aquifer. In this area, groundwater flowing toward the south moves upward where it meets groundwater with higher salinity. To the south, leakage is downward into the aquifer. The Buttonwood Embankment, which is a narrow ridge that separates the wetlands from Florida Bay, impedes surface water flowing south and increases wetland stage levels slightly higher than stage levels in Florida Bay. South of the Buttonwood Embankment, groundwater discharges upward into the coastal embayments of Florida Bay. This upward leakage in the model is caused by the higher water levels on the north side of the embankment. These model results suggest that surface water and groundwater interactions are an important component of the water budget for the Taylor Slough area.



Base from U.S. Geological Survey digital data, 1972
Albers Equal-Area Conic projection, Datum NAD 1983
Standard Parallels 29°30′ and 45°30′, central meridian 23°00′

Figure 2: Map of southern Florida showing SICS model domain and simulated values of leakage between surface water and groundwater.

3. MOCDENS3D

Gualbert Oude Essink

3.1 Program Description

The computer code MOCDENS3D [Oude Essink, 1998, 2001] can simulate groundwater flow and coupled solute transport in porous media. The code is based on the United States Geological Survey public domain three-dimensional finite difference computer code MOC3D [Konikow et al., 1996]. Density differences in groundwater are taken into account in the mathematical formulation. So-called freshwater heads and buoyancy term are introduced. As a result, it is possible to simulate non-stationary flow of fresh, brackish and saline groundwater in coastal aquifers. In chapter X? of this salt water intrusion book, the characteristics of this numerical code are described in detail. Note that MOCDENS3D is similar to SEAWAT: the first uses MOC3D for solute transport, whereas the latter applies MT3DMS [Zheng and Wang, 1999].

3.2 Effect of Sea Level Rise and Land Subsidence in a Dutch Coastal Aquifer

3.2.1 Introduction to the Dutch situation

Salt water intrusion is threatening coastal groundwater systems in the Netherlands. At the root of the problem are both natural processes and anthropogenic activities that have been going on for centuries. Autonomous events, land subsidence and sea level rise all influence the distribution of fresh, brackish and saline groundwater in Dutch coastal aquifers.

The greatest land subsidence is occurring in the peaty and clayey regions in the west and north of the Netherlands and emanates from two, human-driven processes. The first – soil drainage – is a slow and continuous process that started about a thousand years ago when the Dutch began to drain their swampy land. The second – land reclamation – causes a relatively abrupt change in the surface level. In particular, it was the reclamation of the deep lakes during the past centuries that caused the strong flow of saline groundwater from the sea to the coastal aquifers. These so-called *polders* are currently experiencing upward seepage flow.

An example of a Dutch coastal aquifer will show that on the long term, the effects of sea level rise and land subsidence – in terms of the amount of seepage, average salt content and salt load – can be considerable [Oude Essink and Schaars, 2003]

3.2.2 Model of the groundwater system of Rijnland Water Board

The Rijnland Water Board has a surface area of about 1100 km^2 (Fig. 3a) and accommodates some 1.3 million people. Already since the 12th century, the water board manages water quantity and water quality aspects in the area. Sand dunes are present at the western side of the water board (Fig. 3b). Three major drinking water companies are active in the dunes:

DZH (Drinking water company Zuid-Holland), GWA (Amsterdam Waterworks) and PWN (Water company Noord-Holland).

Phreatic water levels in the dune-areas can go up to more than 7 meters above mean sea level. At the inland side of the dune area, some large low-lying polder areas with controlled water levels occur (Fig. 4a). The lowest phreatic water levels in the water board itself can be found northwest of the city Gouda (down to nearly -7 m M.S.L.) and in the Haarlemmermeer polder, where the airport Schiphol is located, with levels as low as -6.5 m M.S.L. Before the middle of the 19th century, a lake covered the Haarlemmermeer polder area. Due to flooding threats at the neighbouring cities, this lake was reclaimed during the years 1840-1852 which caused a relative abrupt change in heads. Subsequently, a completely different groundwater flow regime was created regionally. In addition, the polder Groot-Mijdrecht, situated outside the water board, is also mentioned here. Though the surface area of this polder is not large, the phreatic water level is low (less than -6.5 m M.S.L.) and the Holocene aquitard on top of the groundwater system is very thin. Seepage in this area is very large (more than 5 mm/day) and groundwater from a large region around it is flowing to the polder at a rapid pace. Some large groundwater extractions from the lower aquifer system are taking place, up to 20 million m^3/yr at Hoogovens near IJmuiden.

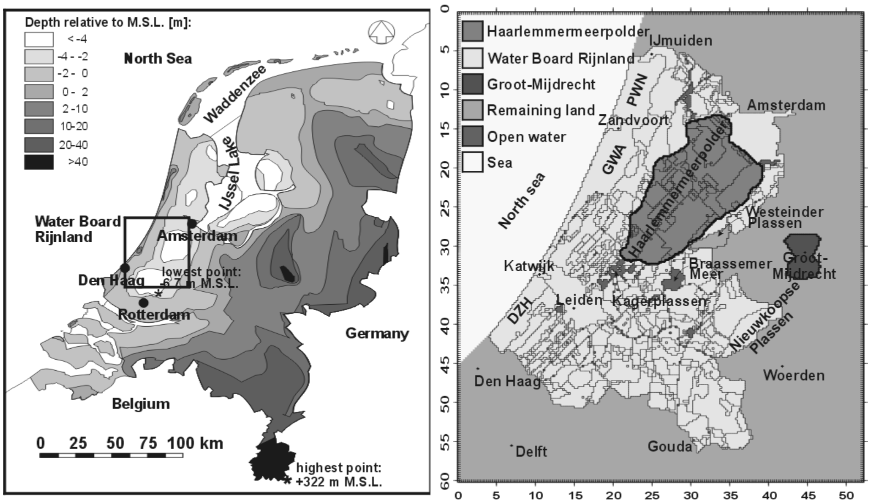


Figure 3: a. Map of The Netherlands: position of the Rijnland Water Board and ground surface of the Netherlands; b. Map of the Rijnland Water Board: position of some polder areas and the sand-dune areas of the drinkingwater companies DZH, GWA and PWN. The Haarlemmermeer polder is also a part of the water board.

The groundwater system consists of a 3D grid of 52.25 km by 60.25 km (~3150 km^2) by 190 m depth and is divided into a large number of elements. Each element is 250 m by 250 m in horizontal plane. In vertical direction the thickness of the elements varies from 5 m for the ten upper layers to 10 m for the deepest fourteen layers (Fig. 4b). The grid contains some 1.2million active elements: n_x=209, n_y=241, n_z=24, where n_i denotes the number of elements in the *i* direction. Each element contains initially eight particles, which gives in total 9.6 million particles to solve the advection term of the solute transport equation. The flow time step Δt to recalculate the groundwater flow equation is one year. The convergence criterion for the groundwater flow equation (freshwater head) is equal to 10^{-4} m.

Data has been retrieved from NAGROM (The National Groundwater Model of The Netherlands). Fig. 4b shows the composition of the groundwater system into three permeable aquifers, intersected by an aquitard in the upper part of the system and an aquitard of clayey and peat composite between -70 and -80 m M.S.L. For each subsystem, the interval of the used horizontal hydraulic conductivity k_h is given in the figure. The anisotropy ratio k_v/k_h is assumed to be 0.1 for all layers. The effective porosity n_e is a bit low: 25%. The longitudinal dispersivity α_L is set equal to 1 m, while the ratio of transversal to longitudinal dispersivity is 0.1.

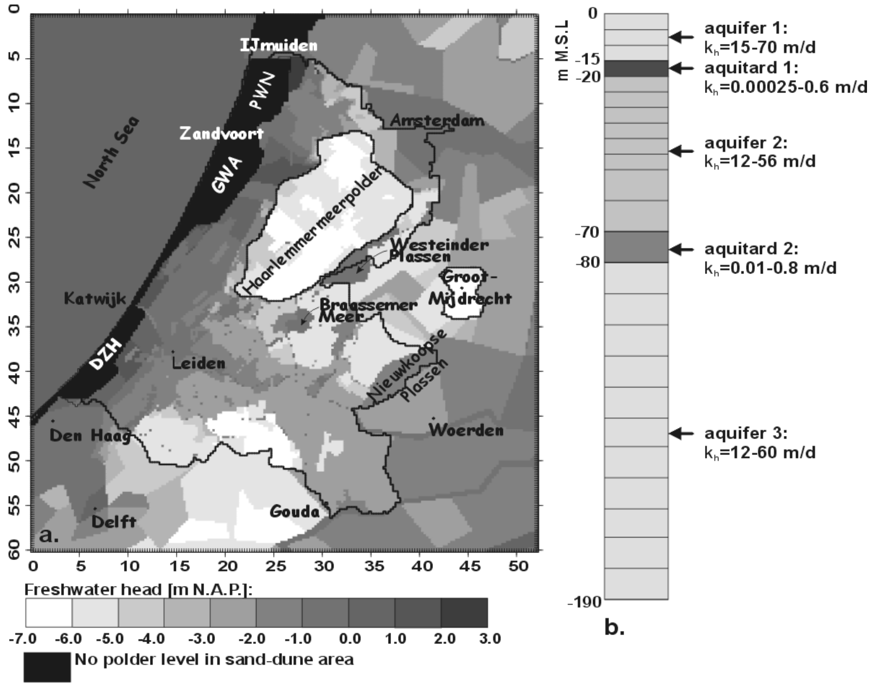


Figure 4: a. Phreatic water levels or polder levels in the area (note that in the sand-dune areas, no polder levels are given); b. Simplified subsoil composition of the bottom of the water board of Rijnland and hydraulic conductivity values.

The bottom of the system is a no-flow boundary. Hydrostatic conditions occur at the four sides of the model. At the top of the system, the natural groundwater recharge in the sand-dune area varies from 0.94 to 1.14 mm/day. The water level at the sea is set to 0.0 m M.S.L. for the year 2000 AD. The general head boundary levels in the polder area are equal to the phreatic water level in the considered polders units, varying from +2.0 m near IJmuiden to -7.0 m M.S.L. northwest of Gouda.

At the initial situation (2000 AD), the hydrogeologic system contains saline, brackish as well as fresh groundwater. On the average, the salinity increases with depth, whereas freshwater lenses exist at the sand-dune areas at the western part of the water board, up to -90 m M.S.L. Fresh water from the sand-dunes flows both to the sea and to the adjacent low-lying polder areas. The chloride concentration of the upper layers is already quite high in some low-lying polder areas such as the Haarlemmermeer polder and the polder Groot-Mijdrecht. The volumetric concentration expansion gradient β_C is 1.34 x 10^{-6} l/mg Cl^-. Saline groundwater in the lower layers does not exceed 18630 mg Cl^-/l. The corresponding density of that saline groundwater equals 1025 kg/m^3.

Calibration was focused on freshwater heads in the hydrogeologic system, and to some extent on seepage and salt load values in the Haarlemmermeer polder and the polder Groot-Mijdrecht. Calibration data has been derived from the water board itself, the NAGROM database, ICW (1976) and the DINO database of Netherlands Institute of Applied Geosciences (TNO-NITG). The model was calibrated by comparing 1632 measured and computed freshwater heads, and for seepage and salt load values of some polders. Note that the measured heads are corrected for density differences. The mean error between measured and computed freshwater heads is -0.16 m, the mean absolute error 0.61 m and the standard deviation 0.79 m.

3.2.3 Sea level rise and land subsidence

It is expected that climate change causes a rise in mean sea level and a change in natural groundwater recharge. As exact figures are not known yet, an average impact scenario is considered here by taking into account the most likely future developments in this area:

- According to the Intergovernmental Panel of Climate Change [IPCC, 2001], a sea level rise of 0.48 m is to be expected for the year 2100 (relative to 1990), with an uncertainty range from 0.09 to 0.88 m. Based on these figures, a sea level rise of 50 cm per century will be implemented at the North Sea, in steps of 0.005 m per each time step of one year, for 2000 AD on,
- An instantaneous increase of natural groundwater recharge at all sand-dune areas of 3% at 2000 AD,
- Oxidation of peat, compaction and shrinkage of clay, and groundwater recovery are causing land subsidence, especially in the

peat areas of the water board. The following values are inserted: a land subsidence of -0.010 m per year for the peat areas; no subsidence for the sand-dune areas; and -0.003 m per year for the rest of the land surface (respectively approximately 25%, 9% and 66% of the land surface in the entire modelled area),

- A reduction of groundwater extraction in the sand-dune areas GWA (-1.3 million m3/yr) and PWN (-4.5 million m3/yr).

The total simulation time is 200 years.

3.2.4 Discussion of results

The overall picture is that the groundwater system will contain more saline groundwater these coming centuries. The numerical model supports the theory that the present situation is not in equilibrium from a salinity point of view. Fig. 5 shows the chloride distribution at –2.5 and –47.5 m M.S.L. for the years 2000 and 2200 AD. Salinisation [GOE: Salinization is US-English?, and thus more consistent woth other text? If yes, change every ‘salinisation’ to ‘salinization’] is going on, especially in the areas close to the coastline. Though the differences might look small due to the fact that groundwater flow and subsequently solute transport are slow processes, changes in seepage and salt load at the top aquifer system are pretty significant (Fig. 6). The combination of autonomous development (reclamation of the deep lakes in the past), sea level rise and land subsidence will intensify the salinisation process: partly due to an increase of seepage values (+6% in 2050 and +12% in 2200, relative to now) but mainly due to the increase in salinity of the top aquifer system. As a result, the overall salt load in the water board is estimated to increase +38% in 2050 and even +79% in 2200, relative to now. The more rapid increase in salt load is caused by an increased salinisation of the upper aquifers.

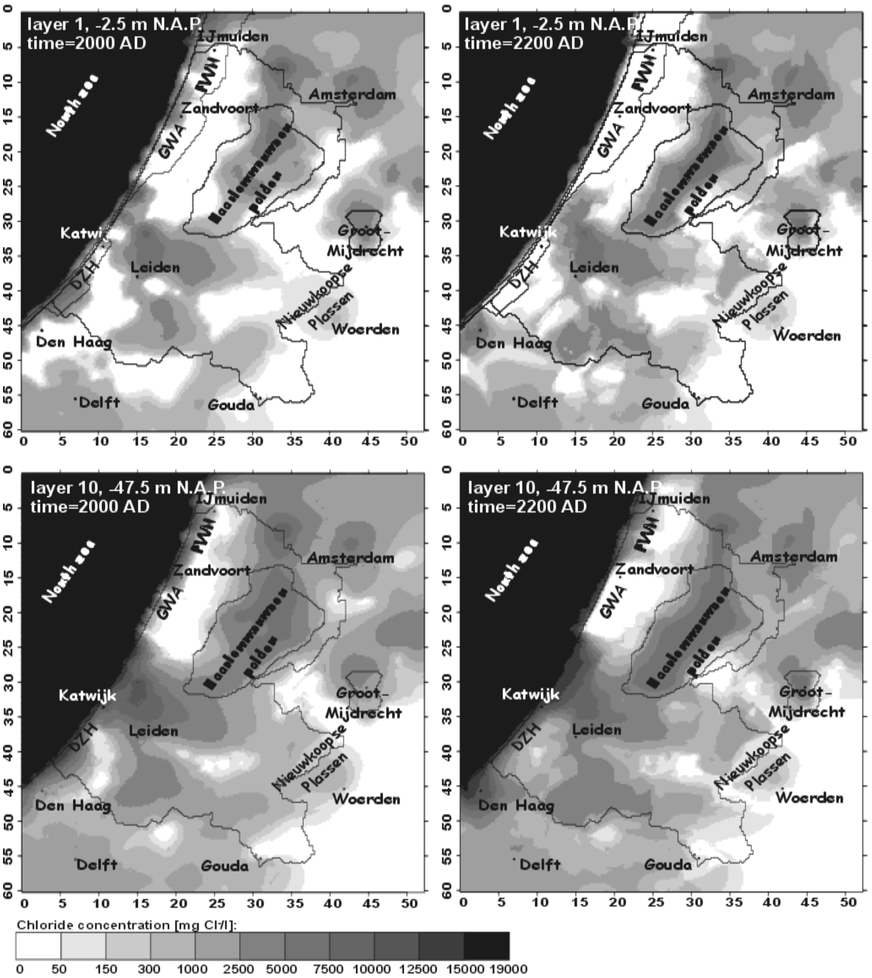


Figure 5: Chloride concentration at –2.5 and –47.5 m M.S.L. for the years 2000 and 2200 AD. Sea level rise and land subsidence is considered.

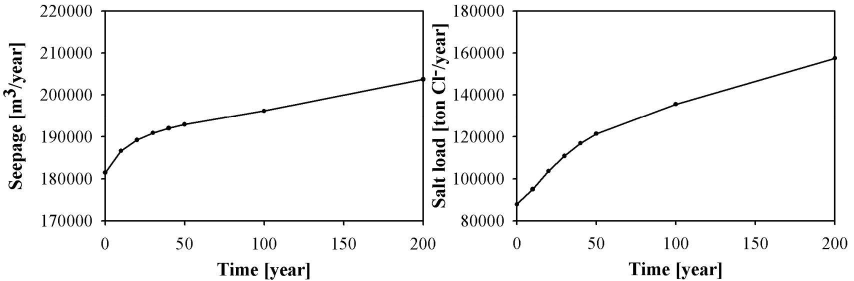


Figure 6: Seepage (in m^3/day) and salt load (in ton Cl$^-$/year) through the second model layer at –10 m M.S.L., summarised for the entire Rijnland Water Board, as a function of 200 years.

3.2.5 Conclusions

A model of the variable density groundwater flow system of the Rijnland Water Board is constructed to quantify the effect of anthropogenic activities, climate change (rise in sea level and an increase in natural groundwater recharge in the sand-dune areas), and land subsidence in large parts of the water board. The code MOCDENS3D is used to simulate density dependent groundwater flow under influence of the above mentioned stresses. Numerical computations indicate that a serious salt water intrusion can be expected during the coming decennia, mainly because a large part of the Rijnland Water Board is lying below mean sea level. The combined effect will be for 2050 AD: a 6% increase of seepage and a 38% increase of salt load in the Rijnland Water Board. The increase in especially salt load will definitely affect surface water management aspects at the water board.

4. MODHMS

Sorab Panday, Walter Jones, Michael Beach, Mark Barcelo

4.1 Program Description

4.1.1 Description

MODHMS [HydroGeoLogic, 2002] is a comprehensive hydrologic modeling system that extends MODFLOW to include the unsaturated zone, the overland flow domain, and channel/surface-water features. Contaminant transport routines are also incorporated for fate and transport calculations in single or dual porosity systems. Density coupling of the flow-field with concentrations of some or all species provides comprehensive analysis capabilities for complex coastal issues.

4.1.2 Physical Concepts and Model Features

MODFLOW's capabilities are expanded by MODHMS to solve the Richards equation for three-dimensional saturated-unsaturated subsurface flow, coupled with the diffusive wave equations for two-dimensional overland and one-dimensional channel flow (including effects of scale, pond storage, routing, and hydraulic structures). The primitive form of the transport equation for single or multiple species is also solved, with optional dual porosity considerations for the subsurface. Nonlinear adsorption and linear decay processes are incorporated, with provisions to accommodate user-supplied, complex reaction modules. Multi-phase transport occurs with equilibrium partitioning considerations and diffusion/storage/decay in the inactive (air) phase. Non-isothermal conditions may be simulated by allocating the temperature variable as the first species of solution. Density coupling (in surface and subsurface regimes) of flow with transport of some or all contaminant species is achieved via a linear density relationship with concentration (adjustment of viscosity and density for the conductance term may also be optionally applied). Fluid pressure is therefore affected by species concentration, and the advection and dispersion terms are affected by the resultant volumetric fluid fluxes. Various combinations of the above simulation capabilities may be used for optimal solution to a given problem.

In addition to MODFLOW's stress packages, MODHMS includes fracture-wells to handle multi-layer pumping and prevent overpumping; an unconfined recharge seepage-face package (for subsurface simulations only) for ponding and hillslope seepage issues; and a comprehensive evapotranspiration (ET) package that accounts for climatic conditions. Transport boundaries include mass fluxes at inflow nodes and prescribed concentrations anywhere in the domain. For density-dependent cases, the flow condition is optionally checked at every iteration or time-step at a constant head node, before applying a prescribed concentration condition.

4.1.3 Computational aspects

The three-dimensional finite-difference grid of MODFLOW is used for subsurface discretization, with a corresponding two-dimensional grid for the overland domain, and a finite-volume discretization for the channel/surface-water body domain. Alternatively, an orthogonal curvilinear grid may be used for the overland and subsurface regimes. Surface/subsurface interactions are expressed fully implicitly, or via iterative/linked options. Newton-Raphson linearization may be used for the unsaturated or unconfined flow equations, and pseudo-soil functions (that are more robust for wetting/drying situations) may be used for unconfined systems where unsaturated effects are neglected. The transport equations are solved using mass conserved schemes with Total Variation Diminishing (TVD), upstream or midpoint spatial weighting, and implicit or Crank-Nicolson temporal weighting options. For density-dependent simulations, the flow equation is solved in terms of equivalent freshwater heads, and the density correction is applied via Picard iteration between the flow and transport equations. Adaptive time-stepping and under-relaxation formulas are based on all system non-linearities, for optimal speed and robustness. Solution options are provided for various combinations of transient and steady-state flow and transport analysis.

4.2 Case History

4.2.1 Site Location and Project Objectives

The study area lies in the southern portion of the Southwest Florida Water Management District (SWFWMD). The model domain includes all or portions of Pinellas, Hillsborough, Manatee, and Sarasota Counties and extends into the Gulf of Mexico covering approximately 60 miles by 100 miles (Fig. 7). Management of saltwater intrusion due to significantly increased groundwater withdrawals was investigated using a density-dependent MODHMS model. Boundary conditions and model parameters were derived from a larger, regional MODFLOW model developed by the SWFWMD and referred to as the Southern District (SD) model. The local model was calibrated to available chloride and water level information from pre-development to current conditions. A steady-state pre-development calibration provided assumed hydrostatic equilibrium behavior of the flow/transport system under long-term average recharge conditions, and was followed by a post-development transient simulation using pumping estimates throughout the study area, from 1900 to 2000. The calibrated model was used to predict the impact of several potential water management scenarios from current conditions to 2050. Results of this analysis assisted in the development of a water level index that will aid in long-term management of groundwater resources. The attached CD contains the detailed report of this study [HydroGeoLogic, 2002].

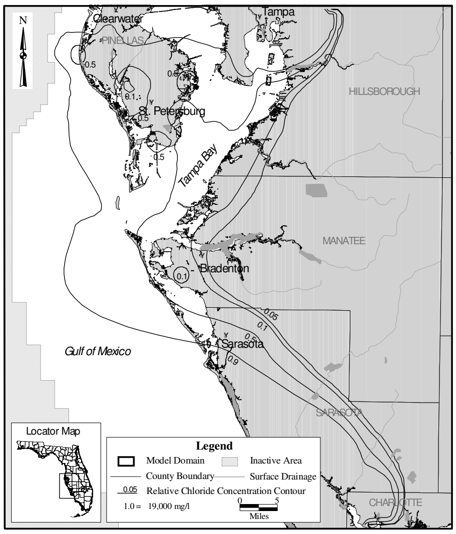


Figure 7: Location of study area and simulated chloride concentrations.

4.2.2 Climate and Hydrogeologic Setting

The site location is humid and subtropical, characterized by warm wet summers and mild dry winters. Long-term rainfall averages 52 in/yr, and mean evapotranspiration is 39 in/yr. The underlying aquifers include the Surficial Aquifer System (SAS), the Intermediate Aquifer System (IAS), and the Floridan Aquifer System (FAS) each of which consists of permeable layers separated by lower permeability semi-confining units. The

FAS is subdivided into major units comprising the Upper Floridan Aquifer (UFA), the Middle Confining Unit (MCU), and the Lower Floridan Aquifer (LFA), which is highly saline in this region and not a source of water. The UFA is the principal source of water in the region and is further subdivided into the Suwannee Limestone, the Ocala Limestone, and the Avon Park Formation, which consists of a main water-bearing zone overlying relatively lower-conductivity units. The MCU contains evaporites that are of extremely low conductivity and forms the bottom of the modeled system.

4.2.3 Conceptual Model and Calibration

The density-dependent saltwater intrusion model was developed from the SD model using telescoping mesh refinement, thereby maintaining the hydrostratigraphy, hydrogeologic properties and imposed stresses of the regional model. Hydrogeologic units were further sub-divided vertically in the numerical grid of the local model to provide resolution for saltwater intrusion considerations. Only the FAS was considered for this study, therefore, recharge/discharge from the overlying IAS was obtained from regional flow model results and applied as a general head boundary across the overlying confining unit. The saltwater model domain included the Suwannee Limestone underlain by the Ocala limestone, the Avon Park Formation and the low conductivity Evaporite Zone of the MCU. Chloride and head conditions were prescribed underneath, for provision of upward movement and upconing effects from deeper regions. Hydraulic conductivity values of the various formations were derived from the SD model transmissivity and leakance fields, and landward boundary conditions for each model run were obtained from parallel simulations using the SD model. Vertical anisotropies, dispersivities, and saltwater boundaries were obtained from field estimates or treated as calibration parameters. Conductivity fields were also adjusted slightly.

The model was first calibrated to steady-state environmental heads, and depth-to-chlorides (for 250, 500 and 1000 ppm levels) estimated for predevelopment conditions (early 1900s), with further calibration for transients till the year 2000 (Fig. 8). Calibration measures include collective statistics as well as temporal and depth-dependent heads and chloride concentrations obtained from individual wells. The model was used to predict the effects of different stresses within the SWUCA (400, 600, 800, and 1000 MGD) for the next 50 years, to determine relations between pumping, flow levels, and long-term saltwater intrusion in the FAS.

4.2.4 Model Calibration Results

The MODHMS model was able to accurately simulate hydraulic heads and chloride concentrations within the study area. The calibration to environmental heads was good, and the model adequately represented depth-dependent chloride concentrations (Fig. 8) and chloride movement from pre- to post-development conditions (Fig. 7). Calibration results are also in agreement with qualitative historical data and with previous modeling efforts.

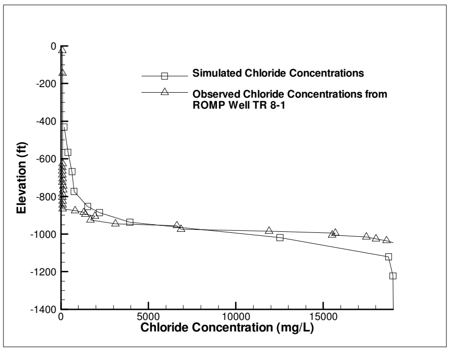


Figure 8: Comparison of observed and simulated chloride concentrations.

5. THE SWI PACKAGE

Mark Bakker

The Sea Water Intrusion (SWI) package is intended for modeling regional seawater intrusion with MODFLOW. The package may be used to simulate the three-dimensional evolution of the salinity distribution, taking density effects into account explicitly. The main advantage of the SWI package is that each aquifer can be modeled with a single layer of cells, without requiring vertical discretization of an aquifer. An existing MODFLOW model of a coastal aquifer can be modified to simulate seawater intrusion with the SWI package through the addition of one input file. The SWI package can simulate interface flow, stratified flow, and continuously varying density flow.

5.1 Theory

The basic idea behind the SWI package is that the groundwater in each aquifer is discretized vertically into a number of zones bounded by curved surfaces. A schematic vertical cross-section of an aquifer is shown in Fig. 9a; the thick lines represent the surfaces. The elevation of each surface is a unique function of the horizontal coordinates. The SWI package has two options. For the *stratified flow* option, water has a constant density between surfaces and the surfaces represent interfaces; the density is discontinuous across a surface (Fig. 9b). For the *variable density flow* option, the surfaces represent iso-surfaces of the density; the density varies linearly in the vertical direction between surfaces and is continuous across a surface (Fig. 9c).

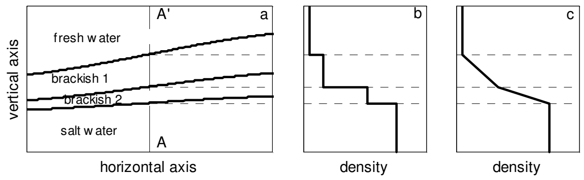


Figure 9: (a) Conceptual model with three surfaces, (b) density distribution of stratified flow, (c) density distribution of variable density flow

Four main approximations are made:

- The Dupuit approximation is adopted and is interpreted to mean that the resistance to flow in the vertical direction is neglected. The Dupuit approximation is accurate for many practical problems of interface flow, even when the slope of the interface is relatively steep (up to 45°), and for variable density flow [Strack and Bakker, 1995]. The vertical pressure distribution is hydrostatic in each aquifer, but this does not mean that there is no vertical flow; the vertical component of flow is computed from three-dimensional continuity of flow.
- The mass balance equation is replaced by the continuity of flow equation in the computation of the flow field (the Boussinesq-Oberbeck approximation); density effects are taken into account through Darcy's law.
- Effects of dispersion and diffusion are not taken into account.
- Inversion is not allowed. Inversion means that saltier (heavier) water is present above fresher (lighter) water, often resulting in the vertical growth of fingers. The SWI package is intended for the modeling of regional seawater intrusion, which is generally on a scale well beyond the size of the fingers.

Dependent variables in the formulation are the freshwater head at the top of each aquifer and the elevations of the surfaces in each aquifer; vertically integrated fluxes. Application of continuity of flow in each aquifer results in a system of differential equations for the freshwater head that is identical in form to the differential equations for single-density flow, but with an additional pseudo-source term, representing the density effects, on the right-hand-side. Hence, MODFLOW can be used to compute the distribution of the freshwater head by addition of this pseudo-source term to the RHS. The differential equations that govern the movement of the surfaces have the same form as the equations for the head, but with different values for the transmissivities and pseudo-source term. Since the form is the same, the solution engines of MODFLOW can again be applied to solve the system for every timestep. A simple tip/toe tracking algorithm is applied to keep track of the horizontal positions of the surfaces. Details of the theory implemented in the SWI package may be found in Bakker [2003].

5.2 Example application

The SWI package is implemented in MODFLOW2000. Only one additional input file is needed to simulate seawater intrusion. The input file consists of the elevations of the surfaces in each aquifer, the density between the surfaces, whether flow should be treated as stratified or variable density, and some tip/toe tracking parameters. MODFLOW/SWI may then be used to compute the positions of the surfaces at the requested times. Details of application of the SWI package may be found in the manual [Bakker and Schaars, 2003]; an executable, manual, and the source code are available for free from the following web page: http://www.engr.uga.edu/~mbakker/swi.html.

One of the major benefits of the SWI package is that it can simulate interface flow, stratified flow, and variable density flow efficiently, even in the same model. Especially when little data is available, it is useful to determine the steady-state position of the interface. This position may already be sufficient to solve the posed problem, or may be used as a starting point for additional transient simulations. When a significant brackish zone is present, the interface may be replaced by one or more brackish zones, either of constant density or variable density. One aquifer may have an interface, while another may have a brackish zone, as will be demonstrated below.

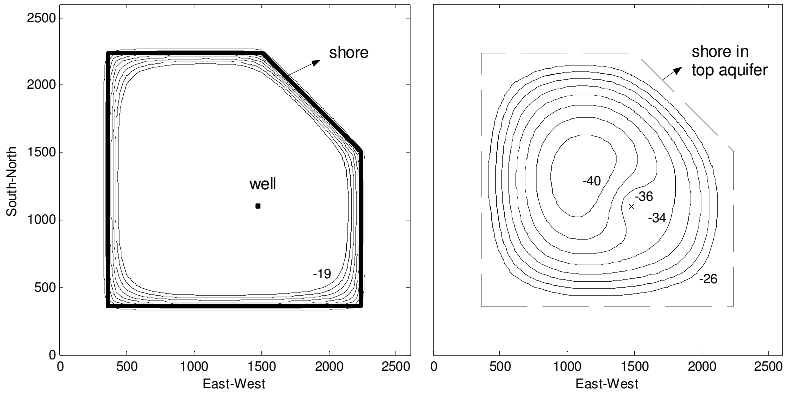


Figure 10: Contours of interface elevation below an island with a well in the top aquifer after 40 years of pumping. Top aquifer (left) and bottom aquifer.

Consider seawater intrusion below the hypothetical five-sided island shown in Fig.10. The top aquifer extends from 0 to –20 m, and has a transmissivity of 100 m^2/d; the bottom aquifer extends from –25 to –55 m, and has a transmissivity of 150 m^2/d. The leakance (V_{cont}) of the leaky layer is 0.002 d^{-1}. The island is surrounded by the ocean, with a fixed level of 0 m; the vertical leakance of the bottom of the ocean, representing the vertical resistance to outflow into the ocean, is 0.1 d^{-1}. Recharge on the island is 0.5 mm/d and is specified with the RCH package. The effective porosity of both aquifers is 0.2. The freshwater heads are computed assuming consecutive steady-state conditions, as the heads will react much quicker than the position of the interface; heads can be treated as transient as well, but modeling them as consecutive steady-states has little influence on the results and allows for the specification of much larger timesteps.

The island is discretized into cells of 25 by 25 meters; the grid is extended at least 350 m into the ocean in all directions. The ocean cannot be modeled with GHB cells, as all sinks and sources in the SWI package are treated as consisting of freshwater. The ocean is modeled with an additional layer on top of the model, consisting of inactive cells wherever the island sticks out of the ocean, and fixed head cells elsewhere. Surfaces or interfaces will be specified at the top of the additional layer, such that all water is salt. The vertical leakance between the additional layer and the first aquifer represents the leakance of the ocean bottom.

As a first step in the modeling process, flow is treated as interface flow. The saltwater has a density of 1025 kg/m^3. The maximum slope of the interface is specified as 0.03, and the other two tip/toe tracking parameters are specified according to the guidelines in the SWI manual. The steady-state position of the interface is approached after 80 steps of 250 days, starting from a rough first guess. The freshwater zone in the bottom aquifer is over 18 m thick in the middle of the island. The steady-state position is used as a starting point for further modeling. A well is started in the top aquifer and has a discharge of 200 m^3/d (about 10% of total recharge on the island). Contours of the elevation of the interface after 40 timesteps of 1 year are shown in Fig.10. The well has little effect on the position of the interface in the top aquifer, but there is an upcoming of 8 meters below the well in the bottom aquifer.

As it is crucial for the saltwater to remain in the bottom aquifer and not reach the leaky layer below the well, modeling is continued by replacing the interface in the lower aquifer with a brackish zone, initially extending 5 m above the steady-state position of the interface. The brackish water has a constant density of 1012.5 kg/m^3. The position of the brackish zone along an east-west cross-section through the well is shown after 20 years (dashed) and 40 years (solid) of pumping in Fig.11; results of the interface simulation after 40 years of pumping are also shown in the figure (thick line). It is concluded that the top of a 5 meter thick brackish zone will reach the bottom of the leaky layer after 40 years.

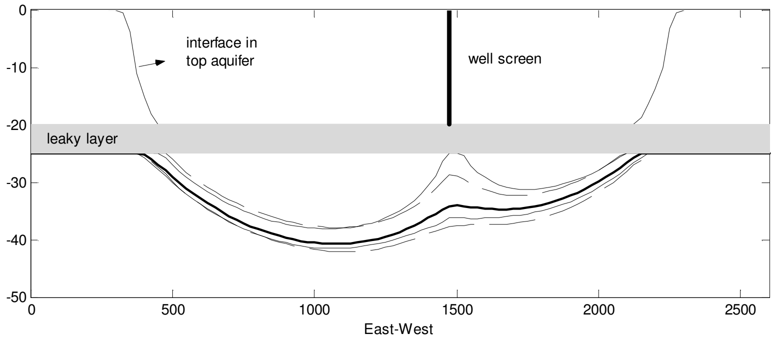


Figure 11: Upconing of brackish zone along east-west cross-section through well. 20 years (dashed), 40 years (solid), interface after 40 years (bold)

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