Proc. of the MODFLOW'98 Conf., Oct. 4-8, 1998, Golden, Colorado, USA, vol. I, pp. 291-303.

MODFLOW'98 Conference

Golden, Colorado, USA, Oct. 4-8 1998

MOC3D adapted to simulate 3D density-dependent groundwater flow

Dr.ir. Gualbert Oude Essink
1. Free University of Amsterdam
Faculty of Earth Sciences
Hydrology and Hydrogeology Department
De Boelelaan 1085
1081 HV AMSTERDAM
The Netherlands
tel.: +31-(0)20-4447265
oudg@geo.vu.nl

2. TNO-NITG (Netherlands Institute of Applied Geosciences)
Grondwater Department
Princetonlaan 6
3584 CB UTRECHT
The Netherlands
tel.: +31-(0)30-2564761
g.oudeessink@nitg.tno.nl

MOC3D adapted to simulate 3D density-dependent groundwater flow

Gualbert H.P. Oude Essink
g.oude.essink@geo.uu.nl
University of Utrecht; Inst. of Earth Sciences;
Centre of Hydrology (ICHU); Dept. of Geophysics;
P.O. Box 80021; 3508 TA Utrecht; The Netherlands

ABSTRACT

The three-dimensional computer code MOC3D (Konikow *et al.*, 1996) is adapted for density differences: MOCDENS3D. As a result, it is possible to model transient three-dimensional groundwater flow in large-scale hydrogeologic systems where non-uniform density distributions occur. A special field of application is the simulation of salt water intrusion in coastal aquifers. The groundwater flow equation is solved by the MODFLOW module of MOCDENS3D. Density differences are taken into account through adding buoyancy terms to the RHS term of the basic groundwater flow equation of MODFLOW. The advection-dispersion equation is solved by the MOC module, using the method of characteristics. Advective transport of solutes is modeled by means of particle tracking and dispersive transport by means of the finite difference method. An advantage of applying the method of characteristics is that the condition of spatial discretisation is not strict. As a consequence, the displacement of fresh, brackish and saline groundwater in large-scale hydrogeologic systems can easily be modeled. Finally, the evolution of a freshwater lens at a circular sandy island is shortly discussed.

INTRODUCTION

Developments in the field of computer codes for simulating 3D density dependent groundwater are advancing rapidly. Several 3D codes, such as HST3D (Kipp, 1986), SWICHA (Huyakorn *et al.*, 1987), METROPOL (Sauter, 1987), SWIFT (Ward, 1991), FEFLOW (Diersch, 1994), are already capable of simulating complex geometries, whereas other codes are in a (final) testing phase such as MVAEM[1] (Strack, 1995) and FAST-C 3D (Holzbecher, Bear *et al,* 1998). Nevertheless, still substantial restrictions remain. For instance, when geometries are large-scale, viz. at least several hundreds of square kilometres by a few hundreds metres depth, sophisticated hardware such as a UNIX background and many tens to hundreds of Mb's Extended Memory is still required to cope with the enormous number of elements. Moreover, there is the perpetual data availability problem, since 3D modeling needs a large amount of data sets for calibration and verification whereas reliable data sets are in practice rare. As such, it has to be accepted that

[1] Note that the code MVAEM still neglects the process of hydrodynamic dispersion, as only advection is taken into account. This is probably not allowed when large time periods are considered or when groundwater velocities are substantial (e.g. in case of high extraction rates of groundwater).

data collection will always lag behind the developments in computer possibilities (Oude Essink & Boekelman, 1996).
In this paper, a new computer code for three-dimensional density dependent groundwater is presented, which is based on the computer code MOC3D (Konikow *et al.*, 1996). Note that the Testing and Research Institute of the Netherlands Waterworks (KIWA) is simultaneously developing a combination of MODFLOW (adapted for density differences) and the solute transport code MT3D96 (Schaars, 1996; Van Gerven & Schaars, 1998, see also this MODFLOW'98). It is relatively easy to adapt MOC3D, from now on called MOCDENS3D, in order to model transient 3D density dependent groundwater flow. An important feature of this code is that it can model large-scale geometries by using coarse elements without causing severe numerical implications. In this setup, also hydrodynamic dispersion is taken into account.
The code can simulate transient groundwater flow of fresh, brackish and saline groundwater in coastal areas where non-uniform density distributions occur. For instance, the code can be applied to optimize sustainable groundwater extraction rates in favour of drinking water supply in coastal aquifers where upconing of saline groundwater is possible. Note that, in addition, normal computations can still be executed with 'ordinary' solute transport without density differences, such as the displacement of contaminations through the subsoil.
In this paper, the most important features of MOCDENS3D are shortly discussed. In addition, the basic finite difference equation of the MODFLOW module, adapted for density differences, is derived by applying so-called freshwater heads. A problem on the evolution of a freshwater lens in a 3D phreatic aquifer, schematised by a sharp interface between fresh and saline groundwater, is shortly discussed. Finally, some conclusions are drawn.

CHARACTERISTICS OF MOCDENS3D

MOCDENS3D (in total some 15000 FORTRAN lines including remarks), which is in fact MOC3D (Konikow *et al.*, 1996) but now adapted for density differences, consists of two robust modules which are fully integrated with each other. First, it comprises a solute transport module, here called the MOC module[2], to displace the density field (originally, this module was applied to simulate ordinary solute transport). Second, it comprises a groundwater flow module, here called the MODFLOW module[3], adapted for density differences to compute transient density dependent groundwater flow. This feature is possible by inserting a so-called buoyancy term in the basic equation of the MODFLOW module, a relatively simple adaptation as can be seen in the following section. The velocity field distribution is derived from the computed freshwater head distribution. Subsequently, the velocity field is used in the MOC module to simulate changes in density field. As such, the two modules are coupled with each other. Some characteristics of MOCDENS3D are:

[2] MOC3D (Konikow, Goode & Hornberger, 1996), version 1.1 of May 1997, is the 3D successor of MOC (Konikow and Bredehoeft, 1978).
[3] The MODFLOW module is just MODFLOW-96 (McDonald and Harbaugh, 1988; Harbaugh and McDonald, 1996), version 3.0 of December 1996, but now fully integrated in MOC3D.

- the code takes into account hydrodynamic dispersion (molecular diffusion as well as mechanical dispersion) and chemical reactions such as adsorption (by means of a retardation factor) and radioactive decay,
- solute transport is modeled through splitting up the advection-dispersion equation into two components: (a) an advective component which is solved by means of a particle tracking technique (the so-called Method Of Characteristics: MOC), and (b) a dispersive component which is solved by the finite difference method. Due to the splitting up, numerical dispersion can be kept within bounds, even if coarse elements and small longitudinal dispersivities are used (Oude Essink & Boekelman, 1996). As such, numerical problems don't occur when elements are measured e.g. 250*250*10 m in combination with a longitudinal dispersivity of α_L=1 m. Especially in this characteristic MOCDENS3D differs from codes which solve the partial differential equations with the standard finite element or finite difference methods. With these methods, severe numerical implications can occur when the spatial discretisation condition is not met. This spatial discretisation condition is characterized by the so-called grid Peclet number[4] (Frind & Pinder, 1982; Daus *et al.,* 1985; Kinzelbach, 1987; Oude Essink & Boekelman, 1996).
- the variation of the pore volume of the elements should be relative small, as otherwise the demand of mass conservation of solute is violated too much[5]. This numerical characteristic is related to the particle tracking technique; as a matter of fact, the 3D solute transport code MT3D (Zheng, 1990) suffers the same problem. In this paper, the applied version of MOCDENS3D uses a uniform grid.
- though numerical dispersion is limited, deviations in the mass balance of solute transport still occur. A substantial difference between the initial mass (in the appearance of the concentration distribution) and the mass after a large number of particle displacements can arise, in particular when discretisation of the elements is coarse or when time steps are large.

ADAPTATION OF THE MODFLOW MODULE FOR DENSITY DIFFERENCES

The discretised continuity equation for a uniform grid in MODFLOW is as follows (McDonald & Harbaugh, 1988):

$$\Sigma Q_i = S_S \frac{\Delta h}{\Delta t} \Delta V \qquad \textbf{(1)}$$

Rewriting this equation in the well-known MODFLOW terms, using the six volume flows Q_i, gives (see the description of the symbols at the end of the paper):

---

[4] The grid Peclet number is defined as $v\Delta x/D_h$, where v=effective velocity [$L\,T^{-1}$], Δx=characteristic length of the element [L] and D_h= hydrodynamic dispersion [$L^2\,T^{-1}$]. At great grid Peclet numbers, e.g. greater than 10 (in theory >2), standard finite element and finite difference methods can cause severe numerical problems, such as non convergence of the solution of the groundwater flow equation, unacceptable numerical dispersion and over- and undershooting of the solute concentration values. Great grid Peclet numbers especially occurs in case of coarse discretisation of large-scale hydrogeologic systems in combination with small longitudinal dispersivities.

[5] As a matter as fact, the density dependent groundwater flow equation in the MODFLOW module could be discretised for elements with a variable pore volume by taking into account density differences in horizontal direction (see e.g. Olsthoorn, 1996). However, elements in the MOC module are considered to be uniform. Therefore, adaptation of density differences in horizontal direction is unnecessary and, as such, not applicable.

$$CV_{i,j,k-1/2}h^{m}_{i,j,k-1} + CC_{i-1/2,j,k}h^{m}_{i-1,j,k} + CR_{i,j-1/2,k}h^{m}_{i,j-1,k} + (-CV_{i,j,k-1/2}$$
$$-CC_{i-1/2,j,k} - CR_{i,j-1/2,k} - CR_{i,j+1/2,k} - CC_{i+1/2,j,k} - CV_{i,j,k+1/2} + HCOF_{i,j,k})h^{m}_{i,j,k}$$
$$+CR_{i,j+1/2,k}h^{m}_{i,j+1,k} + CC_{i+1/2,j,k}h^{m}_{i+1,j,k} + CV_{i,j,k+1/2}h^{m}_{i,j,k+1} = RHS_{i,j,k} \qquad \textbf{(2)}$$

The attention is focused in the vertical volume flow in element i,j,k, see figure 1. First the basic vertical Darcian velocity (specific discharge) is defined as follows (note that the z-axis is pointing downward, as used in MODFLOW):

$$q_z = -\frac{\kappa_z}{\mu}\left(\frac{\partial p}{\partial z} - \rho g\right) \qquad \textbf{(3)}$$

Under normal conditions, MODFLOW applies piezometric heads. However, here so-called freshwater heads[6] are used because density differences are taken into account. Introduction of this freshwater head h_f gives (z-axis is pointing downward):

$$h_f = \frac{p}{\rho_f g} - z \qquad \textbf{(4)}$$

Inserting of eq. (4) in eq. (3) gives:

$$q_z = -\frac{\kappa_z \rho_f g}{\mu}\left(\frac{\partial h_f}{\partial z} - \frac{\rho - \rho_f}{\rho_f}\right) \qquad \textbf{(5)}$$

In many cases small viscosity differences can be neglected if density differences are considered in normal hydrogeologic systems (Verruijt, 1980; Bear & Verruijt, 1987). Equation (5) can then be written as[7]:

$$q_z = -k_z\left(\frac{\partial h_f}{\partial z} - \frac{\rho - \rho_f}{\rho_f}\right) \qquad \textbf{(6)}$$

where $k_z = \kappa_z \rho_f g / \mu$=hydraulic conductivity for fresh water and $(\rho - \rho_f)/\rho_f$=the so-called buoyancy term. Discretisation of this buoyancy term, which is required in the MODFLOW module, gives (see figure 1b):

$$BUOY_{i,j,k} = \left(\frac{(\rho_{i,j,k} + \rho_{i.j.k+1})/2 - \rho_f}{\rho_f}\right) \qquad \textbf{(7)}$$

The MOC module relates the density $\rho_{i,j,k}$ to the solute concentration $C_{i,j,k}$ in groundwater for each element through the equation of state:

$$\rho_{i,j,k} = \rho_f\left(1 + \frac{\rho_s - \rho_f}{\rho_f}\frac{C_{i,j,k}}{C_s}\right) \quad \text{or} \quad \rho_{i,j,k} = \rho_f(1 + \beta C_{i,j,k}) \qquad \textbf{(8)}$$

---

[6] Definition: fictive piezometric head as will be measured when the observation well is filled with fresh groundwater instead of saline or brackish.

[7] Note that in cases with high groundwater densities, such as brine transport in salt domes with densities up to 1200 kg/m^3, eq. (5) instead of eq. (6) should be applied. Moreover, additional cross-coupling terms for Darcy's and Fick's laws are necessary to take into account the dependency of fluid motion to brine transport, and vice versa (e.g. Hassanizadeh and Leijnse, 1988). These terms are not included in MOCDENS3D. As such, under circumstances with high salt concentrations, sophisticated codes such as METROPOL should be applied.

where $C_{i,j,k}$=solute concentration in groundwater in element i,j,k (in mg TDS/l); C_s=reference solute concentration in saline groundwater (e.g. 35000 mg TDS/l); β=coefficient of compositional expansion (e.g.=0.025/35000=7.14≅10^{-7} l/mg TDS). Rewriting eq. (6) in discretised terms of the MODFLOW module and using eq. (7) gives for the flow at the top of element i,j,k:

$$q_{i,j,k-1/2} = -KV_{i,j,k-1/2}\left(\frac{h_{f,i,j,k} - h_{f,i,j,k-1}}{\Delta v_{k-1/2}} - BUOY_{i,j,k-1}\right) \quad \textbf{(9)}$$

and for the flow at the bottom of element i,j,k:

$$q_{i,j,k+1/2} = +KV_{i,j,k+1/2}\left(\frac{h_{f,i,j,k+1} - h_{f,i,j,k}}{\Delta v_{k+1/2}} - BUOY_{i,j,k}\right) \quad \textbf{(10)}$$

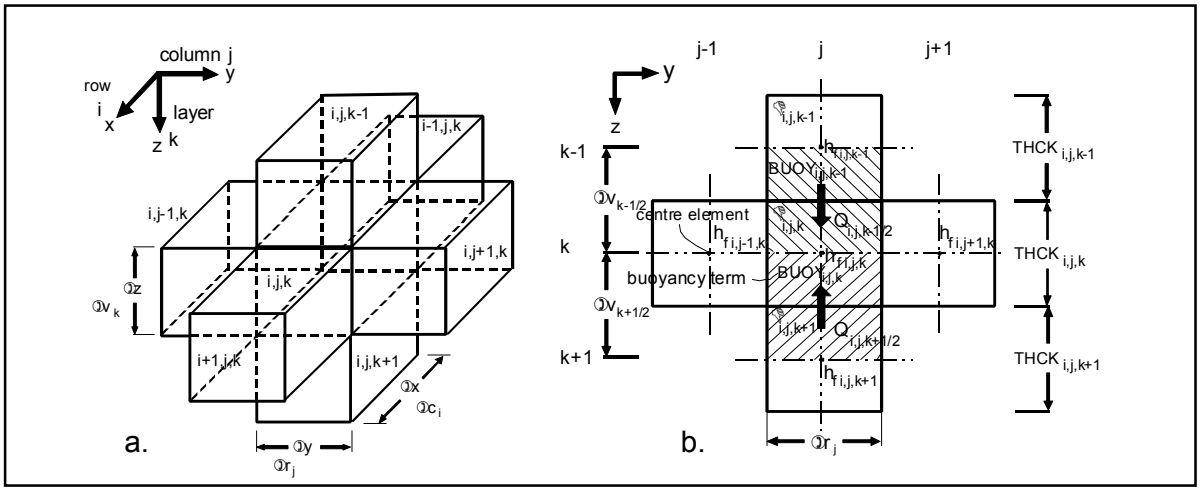

Figure 1: *MODFLOW elements with corresponding density terms.*

The vertical Darcian velocity q is multiplied by the area $\Delta r_j\ \Delta c_i$ to derive the volume flow Q. By using the conductance value in vertical direction, $CV_{i,j,k-1/2} = KV_{i,j,k-1/2}\ \Delta r_j\ \Delta c_i\ /\ \Delta v_{k-1/2}$ (McDonald and Harbaugh, 1988), eq. (9) becomes:

$$Q_{i,j,k-1/2} = +CV_{i,j,k-1/2}\left(h_{f,i,j,k-1} - h_{f,i,j,k} + BUOY_{i,j,k-1}\Delta v_{k-1/2}\right) \quad \textbf{(11)}$$

Similar for eq. (10):

$$Q_{i,j,k+1/2} = +CV_{i,j,k+1/2}\left(h_{f,i,j,k+1} - h_{f,i,j,k} - BUOY_{i,j,k}\Delta v_{k+1/2}\right) \quad \textbf{(12)}$$

As can be seen, in $Q_{i,j,k-1/2}$ the density contribution is positive ($+CV_{i,j,k-1/2}BUOY_{i,j,k-1}\Delta v_{k-1/2}$) whereas in $Q_{i,j,k+1/2}$ it is negative ($-CV_{i,j,k+1/2}BUOY_{i,j,k}\ \Delta v_{k+1/2}$). This is because the direction of flow at the bottom of element i,j,k $Q_{i,j,k+1/2}$ is the opposite to the direction of the z-axis and the gravity. In the MOC module the thicknesses $THCK_{i,j,k}$ of all elements in the grid are known: consequently, $\Delta v_{k-1/2}$ and $\Delta v_{k+1/2}$ can be rewritten as $(THCK_{i,j,k-1}+THCK_{i,j,k})/2$ and $(THCK_{i,j,k}+THCK_{i,j,k+1})/2$, respectively (figure 1b).
Summarizing, three adaptations are necessary to make MOC3D suitable for density dependent groundwater flow:

a. subtract for each element the two buoyancy terms of eq. (11) and (12) from the right hand side term $RHS_{i,j,k}$ in eq. (2) of the MODFLOW module for each time the groundwater flow equation is solved:

$$RHS^{new}_{i,j,k} \Rightarrow RHS^{old}_{i,j,k} - CV_{i,j,k-1/2} BUOY_{i,j,k-1} (THCK_{i,j,k-1} + THCK_{i,j,k}) / 2 + CV_{i,j,k+1/2} BUOY_{i,j,k} (THCK_{i,j,k} + THCK_{i,j,k+1}) / 2 \quad \textbf{(13)}$$

b. add the two buoyancy terms of eq. (11) and (12) to the volume flows $Q_{i,j,k-1/2}$ and $Q_{i,j,k+1/2}$ respectively. These flows are used in the MOC module to simulate solute transport by means of particle tracking:

$$Q^{new}_{i,j,k-1/2} \Rightarrow Q^{old}_{i,j,k-1/2} + CV_{i,j,k-1/2} BUOY_{i,j,k-1} (THCK_{i,j,k-1} + THCK_{i,j,k}) / 2$$

$$Q^{new}_{i,j,k+1/2} \Rightarrow Q^{old}_{i,j,k+1/2} - CV_{i,j,k+1/2} BUOY_{i,j,k} (THCK_{i,j,k} + THCK_{i,j,k+1}) / 2 \quad \textbf{(14)}$$

c. transform piezometric heads h to freshwater heads h_f:

$$h_{i,j,k} \Rightarrow h_{f,i,j,k} \quad \textbf{(15)}$$

As a matter of fact, these adaptations have already been executed by Lebbe (1983) for the 2D solute transport code MOC (Konikow & Bredehoeft, 1978). Note again that h_f has become a fictive freshwater head as density is taken into account. Therefore, streamlines (or velocity vectors) are not perpendicular to the freshwater head contour lines. However, in hydrogeologic systems with ordinary fresh groundwater nothing changes with respect to the original MODFLOW computations.

SIZE OF THE TIME STEP Δt

In case of groundwater flow with variable densities, the velocity field depends on the density distribution through the freshwater head distribution. When fresh, brackish and saline groundwater displace, the density distribution changes accordingly. After a while, the freshwater head distribution and velocity field should be computed once again, as otherwise the velocity field does not correspond with the current density distribution. Consequently, the size of the time step Δt for the groundwater flow equation should be known in advance, since it determines how often the velocity field is computed again. Therefore, it is important to determine the size of the time step Δt. This size depends on the pace of the solute process involved as a large time step could cause an unrealistic solution. For instance, the time step Δt in large-scale hydrogeologic systems in coastal dune areas can be in the order of (several) years (Lebbe, 1983; Oude Essink, 1996), whereas near severe groundwater extractions the density distribution can change so fast that a smaller time step is needed (in the order of months). In MOCDENS3D, the size of the time step is manually determined. The so-called CFL (Courant-Friedrichs-Lewy) condition, which is applied by the MOC module for solute transport as a stability criterion (Konikow and Bredehoeft, 1978), could be utilized to estimate an acceptable size of the time step for the groundwater flow equation. The size of the time step is determined on the basis of experience and/or through trial-and-error (e.g. by means of several test computations: when the density distribution changes rapidly, small time steps are required).

BENCHMARK PROBLEMS WITH MOCDENS3D

A benchmark problem for transient 3D density dependent groundwater flow is needed to validate the computer code MOCDENS3D correctly. Unfortunately, no 3D analytical solution is available in which transport of salt by means of advection and hydrodynamic dispersion is considered. It used to be common practice to apply Henry's problem (2D) as a benchmark for groundwater codes which simulate sea water intrusion in coastal aquifers (Henry, 1964). However, it appeared that Henry's analytical solution is not accurate (Segol, 1994). If, however, the benchmark is reduced to a sharp interface between fresh and saline groundwater, then quite a few analytical solutions exist, such as the upconing problem of Bear & Dagan (1964), sharp interface problems in unconfined, confined and semi-confined situations (e.g. Van Dam, 1983) as well as the stationary vertical sharp interface of Verruijt (1980). Note that MOCDENS3D has already been tested for the vertical sharp interface and a fingering problem (Oude Essink, 1998a) as well as for the evolution of a freshwater lens in a one-dimensional aquifer (Oude Essink, 1998b).

EVOLUTION OF A FRESHWATER LENS IN A PHREATIC AQUIFER

In this paper, a transient sharp interface between fresh and saline groundwater in an axial-symmetric phreatic aquifer is used as a 'benchmark'. An analytical solution is derived by Boekelman (1998). He considered a circular sandy island with a freshwater lens evolving due to natural groundwater recharge (see figure 2a).

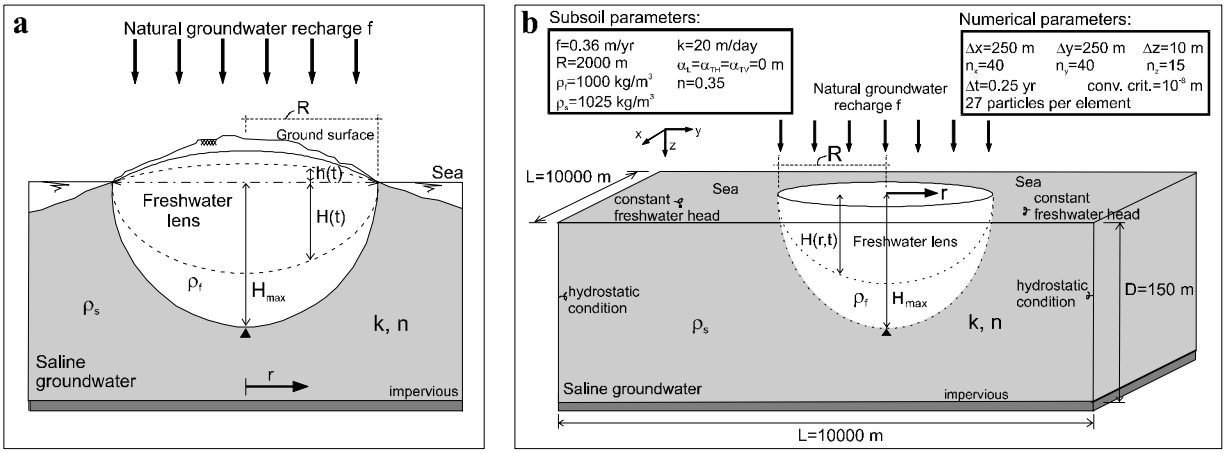

Figure 2: a. *The sharp interface at a circular island*; b. *Schematic representation of the problem.*

The governing equations for this situation are:

Badon - Ghijben Herzberg: $h_f = \alpha H$ **(16)**

Darcy: $$Q = -2\pi r k (H + h_f)\frac{\partial h_f}{\partial r}$$ **(17)**

Continuity: $$\frac{\partial Q}{\partial r} = 2\pi r f - 2\pi r n \frac{\partial H}{\partial t} - 2\pi r n \frac{\partial h_f}{\partial t}$$ **(18)**

Note that eq.(18) comprises two transient terms. Combination of these equations gives:

$$\frac{2n}{k\alpha}\frac{\partial H}{\partial t} = \frac{2f}{k\alpha(1+\alpha)} + \frac{\partial^2 H^2}{\partial r^2} + \frac{1}{r}\frac{\partial H^2}{\partial r} \quad \textbf{(19)}$$

This is not a linear differential equation. Hence, the equation cannot be solved analytically. However, an approximate solution can be found if it is assumed that at each moment the **shape** of the lens is conformable to the shape of the lens in the steady-state situation (t64). If so, the only difference is a time dependent factor F(t). This results in eq. (20):

$$H(r,t) = F(t)\sqrt{\frac{f(R^2 - r^2)}{2k\alpha(1+\alpha)}} \quad \textbf{(20)}$$

$$\text{for } t = \infty: \; F(t) = 1 \text{ (standard analytical solution)} \quad \textbf{(21)}$$

$$\text{for } t = 0: \; F(t) = 0 \quad \textbf{(22)}$$

Eq. (20) is combined with eq. (19) to find the best solution, after which the differential equation is integrated from r=0 to r=R. As a consequence, a solution for F(t) can be found which satisfies the differential equation **on an average**. This leads to the following formula for F(t) (Boekelman, 1998):

$$F(t) = \tanh(t/\tau) \quad \textbf{(23)}$$

$$\text{where:} \quad \tau = \frac{\sqrt{2}\,nR}{3}\sqrt{\frac{(1+\alpha)}{kf\alpha}} \quad \textbf{(24)}$$

The factor τ is a time constant (unit of time) which comprises the characteristics of the geometry. For instance, for $t=\tau$ and 3τ, $\tanh(t/\tau)$.0.761 respectively .0.995.1. This implies that at $t=3\tau$, the shape of the freshwater lens has nearly reached the steady-state situation. Boekelman also derived formulas for the discharge Q and the growth of the freshwater lens. In addition, a similar derivation is given for a one-dimensional elongated island (Boekelman, 1998).
Based on the thickness of the freshwater lens H, the volume of the lens can be determined:

$$V(t) = \pi f R^2 \tau \tanh(t/\tau) \quad \textbf{(25)}$$

The steady-state volume of the freshwater lens (at t64) is equal to:

$$V(\infty) = \pi f R^2 \tau = \frac{\pi\sqrt{2}\,nR^3}{3}\sqrt{\frac{f(1+\alpha)}{k\alpha}} \quad \textbf{(26)}$$

This formula obviously corresponds with the straightforward formula based on the form of the lens: $V=2\pi/3\ n\ (1+\alpha)\ H_{max}\ R^2$, where H_{max}=H(0,4)=maximum depth of the freshwater lens (m). The following parameter set is assumed in this case (figure 2b): α=0.025, R=2000 m, f=0.36 m/yr, k=20 m/day, n=0.35 and $D_{mol}=0\ m^2/s$, $\alpha_L=\alpha_{TH}=\alpha_{TV}=0$ m (no hydrodynamic dispersion). With these values, H_{max}=H(0,4)=62.02 m; the time constant τ=15049 days or 41.20 years and $V(t)=186.4\cong 10^6\cong\tanh(t/\tau)\ m^3$. For the numerical computations the following parameters are applied: 27 particles per element and the convergence criterion for the groundwater flow equation (freshwater head) is equal to 10^{-8} metre. The total simulation time is 400 years. The bottom is impervious whereas at the four sides a hydrostatic condition occurs. At the top of the system, a constant freshwater head exists at the sea and a constant natural groundwater flux at the island. Two sets of discretisation are considered: a) 40*40*15= 24000 elements: Δx=250 m*Δy=250 m*Δz=10 m, Δt=0.25 yr; and b) 100*100*15= 150000 elements: Δx=100 m *Δy=100 m*Δz=10 m, Δt=0.25 yr (since this problem is symmetric in the x-axis as well as the y-axis only 1/4 of geometry could be used for reasons of computational efficiency). At the initial situation,

the aquifer contains only saline groundwater. Figure 3 gives the evolution of the freshwater lens at six moments in time. Though numerical dispersion causes brackish elements, the numerical result corresponds with the analytical solution.

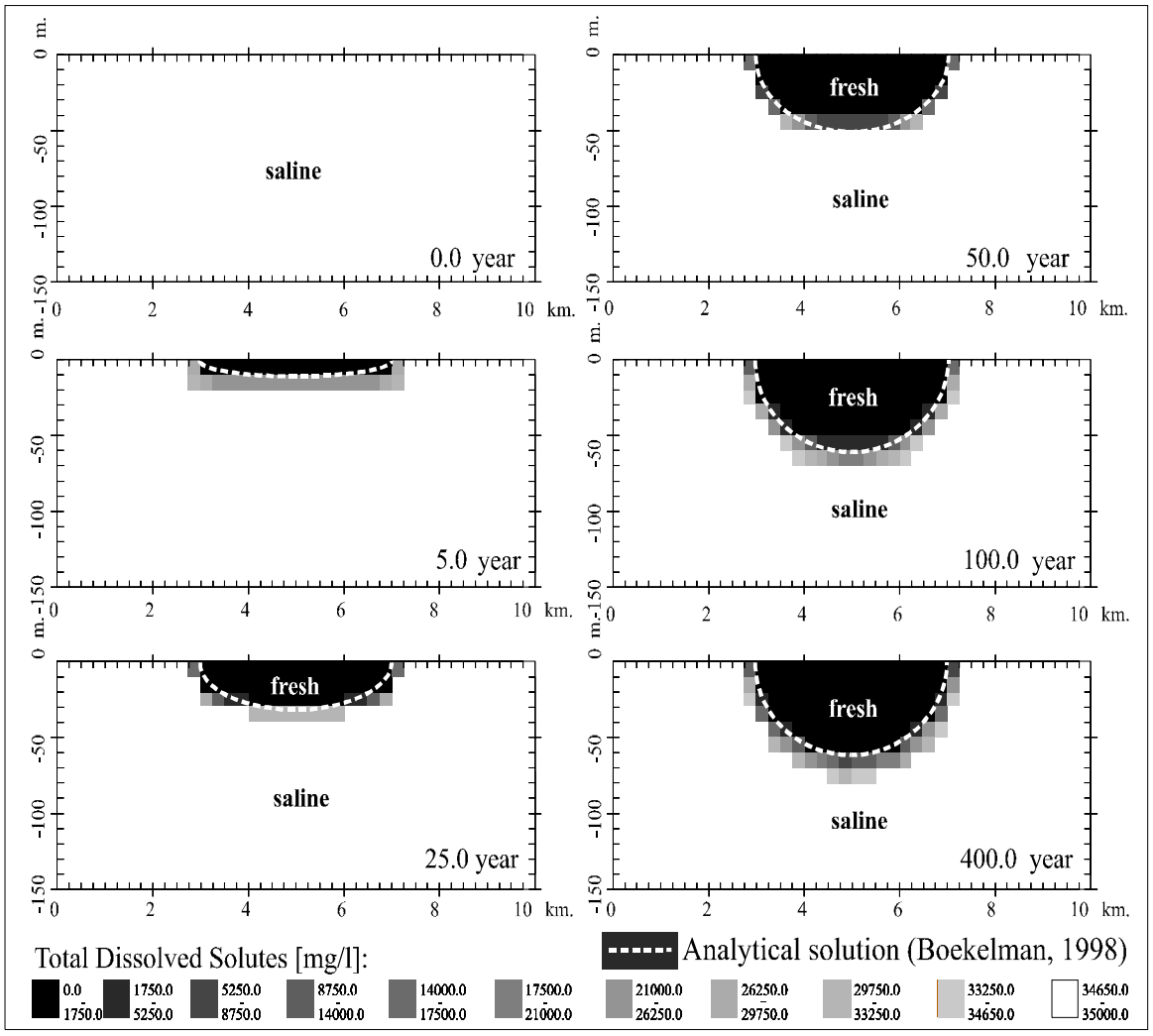

Figure 3: *Evolution of the freshwater lens: transient sharp interface between fresh and saline groundwater for the case with 40*40*15 elements.*

In figure 4, the increase in volume of the freshwater lens can be seen. Note that in this comparison, the volume of the freshwater lens derived by the phreatic part h_f is also taken into account as in the numerical situation the total flux f (=natural groundwater recharge) is inserted in the aquifer. As can be seen, the numerical results approach the analytical solution, though they don't really match each other. This is caused by various reasons. First of all, the analytical solution suggests an aquifer where vertical groundwater flow is neglected, whereas MOCDENS3D simulates vertical groundwater flow as well. This implies that in the numerical computations the outflow of fresh groundwater, equal to $f\pi R^2$, has to exit the aquifer with very

high vertical velocities at the border r=R (total outflow length=2πR). This problem of the outflow of fresh groundwater is not considered in the analytical situation. Second, elements with brackish groundwater are created due to numerical dispersion in the computer code. As a consequence, groundwater near the interface is flowing different than it does in the analytical situation.

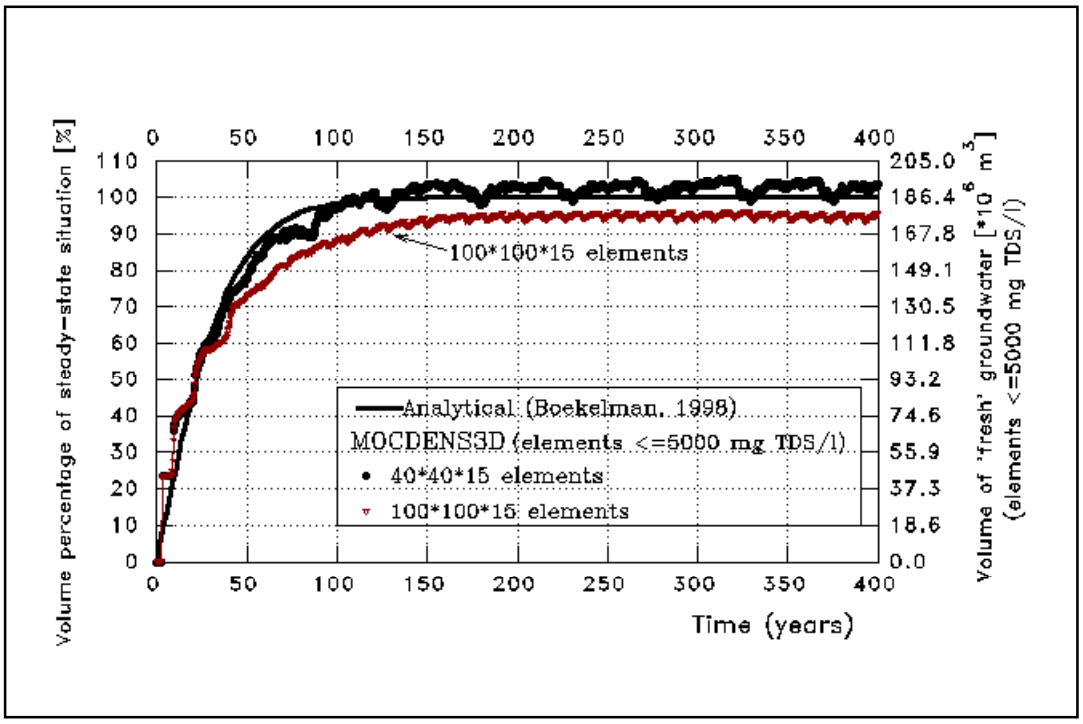

Figure 4: *Evolution of the volume of the freshwater lens. The volume is determined by counting the number of elements with a concentration smaller than 5000 TDS mg/l (e.g. at t=400 year, 882 and 5080 elements <5000 TDS mg/l for discretisation a. and b. respectively).*

CONCLUSIONS

MOCDENS3D can be used to model transient three-dimensional density dependent groundwater flow. The adaptation of the groundwater flow equation of the MODFLOW module is relatively simple. The evolution of a freshwater lens in a phreatic aquifer can be simulated, though substantial numerical dispersion takes place. A proper selection of model parameters such as size of the elements and length of the time step Δt can reduce the error in solute mass balance.

FUTURE DEVELOPMENTS

Recent developments with MODFLOW are impressive. From a geophysical point of view, it is interesting to combine MODFLOW with a code such as RT3D for multi-component transport. As the partial differential equations for solute transport and heat transport are in fact analogous, it could be possible to simulate heat and composition transport in porous media by applying two

components, coupled with the motion of fluid through the equation of state. As a consequence, MODFLOW and RT3D might be applied to simulate groundwater flow in porous media on a continental scale where compositional as well as temperature differences should be taken into account (e.g. double diffusive convection processes).

ACKNOWLEDGEMENT

The author wishes to thank Reinder Boekelman of the Delft University of Technology for applying the analytical solution of the evolution of a freshwater lens in a phreatic aquifer.

COMPUTER ANIMATION OF THE EVOLUTION OF THE FRESHWATER LENS

It is possible to download animations of the evolution of the freshwater lens in the axial-symmetric situation from the following ftp-site: 'ftp://ftp.geo.uu.nl/pub/people/goe'. In addition, the web-site 'http://www.geo.uu.nl/~goe/' can be visited for more information on other research activities of Gualbert Oude Essink.

NOTATION

$C_{i,j,k}$ = solute concentration in groundwater in element i,j,k in mg TDS/l [M L^{-3}]
C_s = reference solute concentration in saline groundwater: e.g. 35000 mg TDS/l [M L^{-3}]
$CC_{i-1/2,j,k}$ = MODFLOW term: horizontal conductance between the elements i-1,j,k and i,j,k [L^2 T^{-1}]
$CR_{i,j-1/2,k}$ = MODFLOW term: horizontal conductance between the elements i,j-1,k and i,j,k [L^2 T^{-1}]
$CV_{i,j,k-1/2}$ = MODFLOW term: vertical conductance between the elements i,j,k-1 and i,j,k [L^2 T^{-1}]
D_{mol} = molecular diffusion [L^2 T^{-1}]
f = natural groundwater recharge [L T^{-1}]
g = gravity [L T^{-2}]
H = thickness of the freshwater lens [L]
H_{max} = H(0,4)=maximum depth of the freshwater lens at r=0 metre and t=4 [L]
$HCOF_{i,j,k}$ = term in the basic equation of MODFLOW for element i,j,k, consisting of terms dependent to the freshwater head h_f [L^2 T^{-1}]
h_f = freshwater head [L]
$KV_{i,j,k-1/2}$ = MODFLOW term: vertical hydraulic conductivity between the elements i,j,k-1 and i,j,k [L T^{-1}]
k = hydraulic conductivity in sand-dune area [L T^{-1}]
k_z = hydraulic conductivity in vertical direction [L T^{-1}]
n = porosity [-]
p = pressure [M L^{-1} T^{-2}]
q_z = vertical Darcian velocity (or vertical specific discharge) [L T^{-1}]
$RHS_{i,j,k}$ = term in the basic equation of MODFLOW for element i,j,k, consisting of terms independent to the freshwater head h_f, such as sources and sinks. In case of density dependent computations the buoyancy terms are added to this term [L^3 T^{-1}]
R = radius of the sand-dune area [L]
S_s = specific storage [L^{-1}]
v = effective velocity [L T^{-1}]
V(t) = volume of the freshwater lens as afunction of time [L^3]
TDS = total dissolved solutes: concentration of dissolved solutes in groundwater in mg/l [M L^{-3}]
$BUOY_{i,j,k}$ = buoyancy term, the relative density difference between the elements i,j,k and i,j,k+1 [-]
z = elevation head (z-axis is pointing vertically downward) [L]
α = relative density difference=$(\rho_s - \rho_f)/\rho_f$ [-]

α_L = longitudinal dispersivity [L]
α_{TH},α_{TV} = transversal dispersivity, respectively horizontal and vertical [L]
β = coefficient of compositional expansion: e.g. $7.14 \cong 10^{-7}$ l/mg TDS [L^3 M^{-1}]
Δh = change in head over a time interval of length Δt [L]
Δc_i = length of element i,j,k in column direction [L]
Δr_j = width of element i,j,k in row direction [L]
Δt = length of the time step to compute again the groundwater flow equation [T]
$\Delta v_{k-1/2}$ = thickness of element i,j,k in layer direction [L]
ΔV = volume of the element [L^3]
κ_z = intrinsic permeability in vertical direction [L^2]
μ = dynamic viscosity [M L^{-1} T^{-1}]
$\rho_{i,j,k}$ = density of groundwater in element i,j,k [M L^{-3}]
ρ_f = density of fresh groundwater: 1000 kg/m^3
ρ_s = density of saline groundwater: 1025 kg/m^3
τ = time constant [T]

REFERENCES

Bear, J. and G. Dagan. 1964. Some exact solutions of interface problems by means of the hodograph method. J. *Geophysical Res., 69 (8): 1563-1572.*

Bear, J. and A. Verruijt. 1987. Modeling groundwater flow and pollution. D. Reidel Publishing Company, Dordrecht, 414 p.

Bear, J., Cheng, A., Sorek, S., Herrera, I. and Ouazar, D. (eds). 1998. Seawater intrusion in coastal aquifers; concept, methods and practices. (In press). Kluwer Academic Publishers.

Boekelman, R.H. 1998. Evolution of a sharp interface in phreatic aquifers. (In press). Communication of the department of water management, environmental and sanitary engineering.

Dam, van, J.C. 1983. The shape and position of the salt water wedge in coastal aquifers. In: *Relation of groundwater quantity and quality. Proc. Hamburg Symp., August 1983, IAHS Publ. no. 146, 59-75.*

Daus, A.D., E.O. Frind and E.A. Sudicky. 1985. Comparative error analysis in finite element formulations of the advection-dispersion equation. *Adv. in Water Resour., 8: 86-95.*

Diersch, H.J.G. 1994. FEFLOW User's manual version 4.2, WASY GmbH, Berlin, Germany.

Frind, E.O. and G.F. Pinder. 1983. The principle direction technique for solution of the advection-dispersion equation. In: *Proc. 10th IMACS World Congress on Systems Simulation and Scientific Computation, Concordia University, Montreal, Canada, Aug. 1982, p. 305-313.*

Gerven, van, M.W. and Schaars, F. The density package, simulation of density driven flow in MODFLOW. (In press). In: *Proc. of the 15th Salt Water Intrusion Meeting, Ghent, Belgium, May 1998.*

Harbaugh, A.W. and M.G. McDonald. 1996. User's documentation for the U.S. Geological Survey modular finite-difference ground-water flow model. U.S.G.S. Open-File Report 96-485, 56 p.

Hassanizadeh, S.M. and T. Leijnse. 1988. On the modeling of brine transport in porous media. *Water Resour. Res., 24 (3): 321-330.*

Henry, H.R. 1964. Effects of dispersion on salt encroachment in coastal aquifers. In: *Sea water in coastal aquifers. Cooper, H.H., jr., Kohout, F.A., Henry, H.R. and Glover, R.E. 84 p. U.S.G.S. Water Supply Paper 1613-C, p. C70-C84.*

Huyakorn, P.S., P.F. Andersen, J.W. Mercer and H.O. White, Jr**.** 1987. Saltwater intrusion in aquifers: development and testing of a three-dimensional finite element model. *Water Resour. Res., 23 (2): 293-312.*

Kinzelbach, W.K.H. 1987. Methods for the simulation of pollutant transport in ground water, a model comparison. In: *Proc. solving ground water problems with models. Conference and Exposition, vol. 1, Denver Colorado, U.S.A., Feb. 1987, p. 656-675.*

Kipp, K.L, Jr. 1986. HST3D: A computer code for simulation of heat and solute transport in three-dimensional groundwater flow systems. IGWMC, International Ground Water Modeling Center, U.S.G.S. Water-Resources Investigations Report 86-4095.

Konikow, L.F., D.J. Goode and G.Z. Hornberger. 1996. A three-dimensional method-of-characteristics solute-transport model (MOC3D). U.S.G.S.Water-Resources Investigations Report 96-4267, 87 p.
Konikow, L.F. and J.D. Bredehoeft. 1978. Computer model of two-dimensional solute transport and dispersion in ground water. U.S.G.S. Techniques of Water-Resources Investigations, Book 7, Chapter C2, 90 p.
Lebbe, L.C. 1983. Mathematical model of the evolution of the fresh-water lens under the dunes and beach with semi-diurnal tides. In*: Proc. of the 8th Salt Water Intrusion Meeting, Bari, Italy, May 1983, Geologia Applicata e Idrogeologia, Vol. XVIII, Parte II: p. 211-226.*
McDonald, M.G. and A.W. Harbaugh**.** 1988. A modular three-dimensional finite-difference ground-water flow model. U.S.G.S. Techniques of Water-Resources Investigations, Book 6, Chapter A1, 586 p.
Olsthoorn, T.N. 1996. Variable density groundwater modelling with MODFLOW. In: *Proc. of the 14th Salt Water Intrusion Meeting, Malmö, Sweden, June 1996, p. 51-60.*
Oude Essink, G.H.P. 1996. Impact of sea level rise on groundwater flow regimes. A sensitivity analysis for the Netherlands. Ph.D. thesis Delft University of technology, Delft Studies in Integrated Water Management: no. 7. (ISBN 90-407-1330- 8). 428 p.
Oude Essink, G.H.P. 1998a. Simuleren van 3D dichtheidsafhankelijke grondwaterstroming: MOCDENS3D. (In Dutch). In: *Stromingen, 4 (1): 5-23.*
Oude Essink, G.H.P. 1998b. Simulating 3D density dependent groundwater flow: the adapted MOC3D. (In press). In: *Proc. of the 15th Salt Water Intrusion Meeting, Ghent, Belgium, May 1998.*
Oude Essink, G.H.P. and R.H. Boekelman. 1996. Problems with large-scale modelling of salt water intrusion in 3D. In: *Proc. of the 14th Salt Water Intrusion Meeting, Malmö, Sweden, June 1996, p. 16-31.*
Sauter, F.J. 1987. User's manual METROPOL; mathematical description. Iterim report no. 728514.002, RIVM, Bilthoven.
Schaars, F. 1996. Implementation of a method for spatial modelling of simultaneous flow of fresh, brackish and saline groundwater in the sand-dune area of Amsterdam Waterworks. (In Dutch). M.Sc. thesis at the Delft University of Technology, the Netherlands. 102 p.
Segol, G. 1994. Classic groundwater simulations. Proving and improving numerical models. Prentice-Hall, Inc. New York. 531 p.
Strack, O.D.L. 1995. A Dupuit-Forchheimer model for three-dimensional flow with variable density. *Water Resour. Res., 31 (12): 3007-3017.*
Ward, D.S. 1991. SWIFT/486: 3-D Model to Simulate Ground-Water Flow, Heat, Brine and Radio Nuclide Transport. GeoTrans, Inc. Sterling, Virginia.
Verruijt, A. 1980. The rotation of a vertical interface in a porous medium. *Water Resour. Res., 16 (1): 239-240.*