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Simulating 3D Density-Dependent Groundwater Flow: the Adapted MOC3D

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ABSTRACT

In this paper, the three-dimensional (3D) computer code MOC3D (KONIKOW et al , 1996) is adapted for density differences: MOCDENS3D As a result, it is possible to simulate transient groundwater flow in large-scale 3D hydrogeologic systems where non-uniform density distributions occur The groundwater-flow equation is solved by a module, which is in fact the MODFLOW computer code. Density differences are taken into account by adding buoyancy terms to the right-hand-side-term of the basic equation of MODFLOW The advection-dispersion equation is solved by the MOC module, using the method of characteristics. An advantage of applying the method of characteristics is that the condition of spatial discretization, characterized by the so-called grid Peclet number, is not strict As a consequence the displacement of fresh, brackish and saline groundwater in large-scale 3D hydrogeologic systems can easily be simulated without severe numerical implications such as non-convergence as well as heavy over- and undershooting In this paper, the evolution of a fresh-water lens in a phreatic aquifer is briefly discussed

INTRODUCTION

Developments in the field of computer codes for simulating 3D density-dependent groundwater flow 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). Nevertheless, there are still some substantial restrictions. For instance, when geometries are large-scaled, viz at least several tens to 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 EM RAM[2] is required to cope with the enormous number of elements. Moreover, there is the perpetual data-availability problem, since 3D modelling 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 data collection (even intensified substantially) 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 flow 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

[1] Note that the code MVAEM neglects the process of hydrodynamic dispersion, as only advection is taken into account This is probably not allowed when long periods are considered or when groundwater velocities are substantial (e g in case of high extraction rates of groundwater)
[2] EM RAM stands for Extended Memory Random Excess Memory

(SCHAARS, 1996; VAN GERVEN & SCHAARS, 1998, see this 15th SWIM) 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 upset, also hydrodynamic dispersion is taken into account The code is capable to simulate transient groundwater flow of fresh, brackish and saline groundwater in coastal areas where non-uniform density distributions occur. Possible applications are simulating the effect on salt-water intrusion into coastal aquifers of natural processes (e.g. sea-level rise) or human activities. Examples of human activities are land reclamation, groundwater extractions for drinking-water supply and lowering of phreatic levels due to land subsidence. Note that, in addition, normal computations can still be executed with 'ordinary' solute transport and no density differences, such as the displacement of contaminations through the subsoil.

In the 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 fresh-water heads A problem about the evolution of a fresh-water lens, schematized 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: (a) a solute-transport module, here called the MOC module[3], to displace the density field (originally, this module was applied to simulate ordinary solute transport); and (b) a groundwater-flow module, here called the MODFLOW module[4], adapted for density differences to compute transient density-dependent groundwater flow This 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 fresh-water head distribution Subsequently, the velocity field is used in the MOC module to model changes in density field. As such, the two modules are coupled with each other. Some characteristics of MOCDENS3D are:

- MOCDENS3D is one computer code which solved the groundwater flow as well as the solute transport equation;
- 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 modelled by splitting the advection-dispersion equation into two components: (a) an adjective component which is solved by means of a particle-tracking technique (the so-called Method Of Characteristics: MOC), and (b) a disperse component, which is solved by the finite-difference method. Due to the splitting, 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 do not occur when elements are sized 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 by the standard finite element or finite-difference methods With these methods, severe numerical implications can occur when the spatial discretization condition is not met. This spatial discretization condition is characterized by the so-called grid Peclet number[5] (FRIND & PINDER, 1982; DAUS et al., 1985; KINZELBACH, 1987; OUDE ESSINK & BOEKELMAN, 1996);

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[3] MOC3D (KONIKOW GOODE & HORNBERGER 1996) version 1 1 of May 1997 is the 3D successor of MOC (KONIKOW & BREDEHOEFT, 1978).

[4] The MODFLOW module is just MODFLOW-96 (McDONALD & HARBAUGH 1988; HARBAUGH & McDONALD 1996), version 3.0 of December 1996 but now fully integrated in MOC3D

[5] The grid Peclet number Pe_{num} 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 Pe_{num}>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 Large grid Peclet num-

- the variation of the pore volume of the elements should be relatively small, as otherwise the demand of mass conservation of solute is violated too much[6] This numerical characteristic is related to the particle-tracking technique; as a matter of fact, the 3D solute-transport code MT3D (ZHENG, 1990) suffers from the same problem. In this paper, the applied version of MOCDENS3D uses a uniform[7] grid;
- though numerical dispersion is limited, deviations in the mass balance of solute transport still occur. A 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 discretization of the elements is coarse and/or when time steps are large.

ADAPTATION OF THE MODFLOW MODULE FOR DENSITY DIFFERENCES

The discretized continuity equation for a uniform grid in MODFLOW is as follows (McDONALD & HARBAUGH, 1988):

$$\Sigma Q_i = S_s \frac{\Delta h}{\Delta t} \Delta V \tag{1}$$

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

$$\begin{aligned} &CV_{i,j,k-1/2} h^m_{i,j,k-1} + CC_{i-1/2,j,k} h^m_{i-1,j,k} + CR_{i,j-1/2,k} h^m_{i,j-1,k} + (-CV_{i,j,k-1/2} \\ &-CC_{i-1/2,j,k} - CR_{i,j-1/2,k} - CR_{i,j+1/2,k} - CC_{i+1/2,j,k} - CV_{i,j,k+1/2} + HCOF_{i,j,k}) h^m_{i,j,k} \\ &+CR_{i,j+1/2,k} h^m_{i,j+1,k} + CC_{i+1/2,j,k} h^m_{i+1,j,k} + CV_{i,j,k+1/2} h^m_{i,j,k+1} = RHS_{i,j,k} \end{aligned} \tag{2}$$

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

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

Under normal conditions, MODFLOW uses piezometric heads. However, here so-called fresh-water heads[8] are used because density differences are taken into account. Introduction of this fresh-water head h_f gives (z-axis is pointing downward):

$$h_f = \frac{p}{\rho_f g} - z \tag{4}$$

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

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

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 [9]:

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bers especially occur in case of coarse discretization of large-scale hydrogeologic systems in combination with small longitudinal dispersivities,

[6] As a matter of fact, the density-dependent groundwater flow equation in the MODFLOW module could be discretized 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.

[7] The length of the element in column direction can differ from the length of the element in row direction.

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

9 Note that in cases with high groundwater densities, e.g. when simulating groundwater in salt domes with densities up to 1200 kg/m3, MOCDENS3D should use eq. (5) instead of eq. (6). In some cases even more sophisticated codes such as METROPOL should be used.

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

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. Discretization of this buoyancy term, which is required in the MODFLOW module, gives (fig. 1b):

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

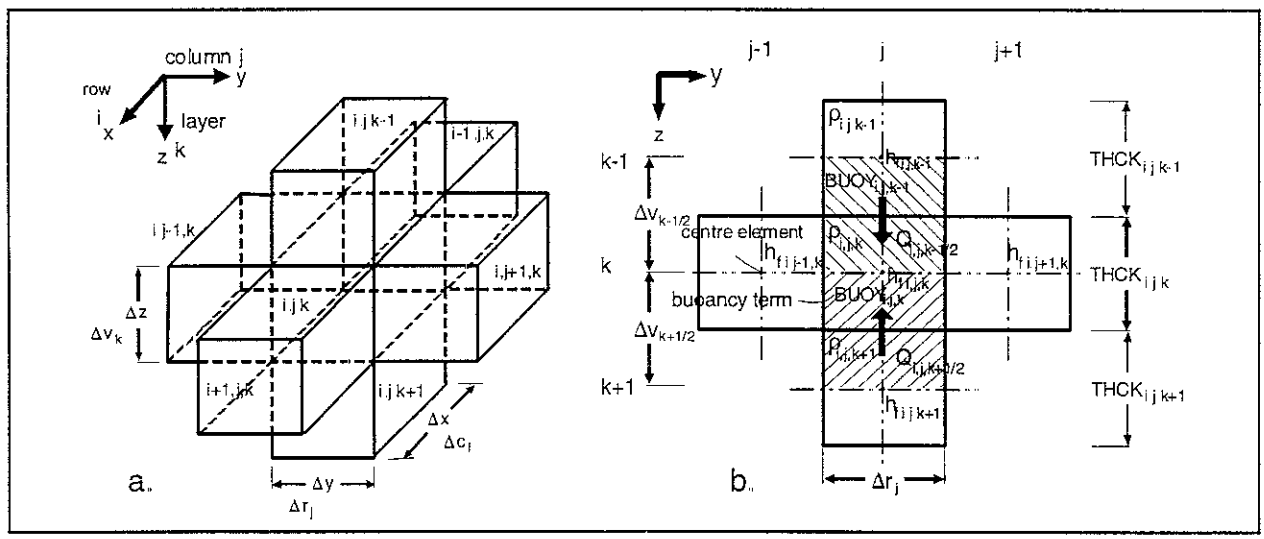

Figure 1. MODFLOW elements with corresponding density terms.

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:

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

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 $\cong 10^{-7}$ l/mg TDS). Rewriting eq. (6) in discretized terms of the MODFLOW module and using eq. (7) gives for the flow at the top of element i,j,k:

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

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

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

The vertical Darcian velocity q is multiplied with the area $\Delta r_j\,\Delta c_i$ to derive the volume flow Q. By using the so-called 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 & HARBAUGH, 1988), eq. (9) becomes:

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

Similar for eq. (10):

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

As can be seen, in $Q_{i,j,k-1/2}$ the density contribution is positive ($+CV_{i,j,k-1/2}BUOY_{i,j,k-1}\Delta v_{k-1/2}$) and in $Q_{i,j,k+1/2}$ 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 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 (fig. 1b).

Summarizing, three adaptations are necessary to make MOC3D suitable for density-dependent groundwater flow:

a. subtract for each time the groundwater-flow equation is solved 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 element:

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

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 model solute transport by means of particle tracking:

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

c. transform piezometric heads h into fresh-water heads h_f:

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

As a matter of fact, these adaptations have already been made by LEBBE (1983) for the 2D solute-transport model MOC (KONIKOW & BREDEHOEFT, 1978). Note again that h_f has become a fictive fresh-water head as density is taken into account. Therefore, streamlines (or velocity vectors) are not perpendicular to the fresh-water head isohypses. 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 with variable densities, the velocity field depends on the density distribution through the fresh-water head distribution. When fresh, brackish and saline groundwater moves, the density distribution changes accordingly. After a while, the fresh-water 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, 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 large 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, could be used 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 by trial-and-error (e.g. by means of several test computations: when the density distribution changes rapidly, smaller time steps are required).

BENCHMARK PROBLEMS WITH MOCDENS3D

In fact, a transient 3D density-dependent groundwater-flow benchmark problem is needed to validate the computer code MOCDENS3D correctly. Unfortunately, a 3D analytical solution, where transport of salt by means of advection and hydrodynamic dispersion is taken into account, is not (yet) available. 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[10] (SEGOL, 1994). If, however, the benchmark is reduced to

[10] This can be is deduced from the fact that no numerical method had succeeded in duplicating Henry's steady-state solution: the analytical solution and the numeric computations always deviate from each other

a sharp interface between fresh and saline groundwater, then quite a few solutions do 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 of VERRUIJT as well as for a fingering problem (OUDE ESSINK, 1998)

In conclusion, analytical benchmark problems for density-dependent groundwater flow are scarce. However, some interesting analytical solutions exist in the field of heat transport in porous media (e.g. TURCOTTE & SCHUBERT, 1982). As the partial differential equations of solute transport and heat transport are analogous, analytical solutions available in heat transport could be transformed to solute-transport problems. An interesting case is that of the convection of heat in porous media (e.g. NIELD, 1968; SCHEIDEGGER, 1974; NIELD & BEJAN, 1992). In this situation, the so-called onset of convection in a porous medium in a conductive environment can be determined analytically, making use of a so-called Rayleigh number[11] Ra. For instance, for a case infinite in horizontal direction, isothermal in terms of heat transport (viz. no heat flux) as well as impermeable in terms of groundwater at $z=\forall 1/2L$, the onset of convection will occur when $Ra>4\pi^2$. Subsequently, convection cells will evolve.

Not really analytical benchmarks, but often applied, are numerical solutions derived in the theory of heat transport in porous media. A famous example is ELDER's fingering problem (1967). He investigated natural (thermal) convection purely driven by fluid-density differences, numerically as well as experimentally. His results were transformed to solute transport in porous media, e.g. by VOSS & SOUZA (1987)

EVOLUTION OF A SHARP INTERFACE IN A PHREATIC AQUIFER

In this paper, a transient sharp interface between fresh and saline groundwater in a one-dimensional phreatic aquifer is used as a 'benchmark'. An analytical solution is derived by BOEKELMAN (1998). He considered an elongated island or strip of sand dunes with a fresh-water lens evolving by natural groundwater recharge (fig. 2a)

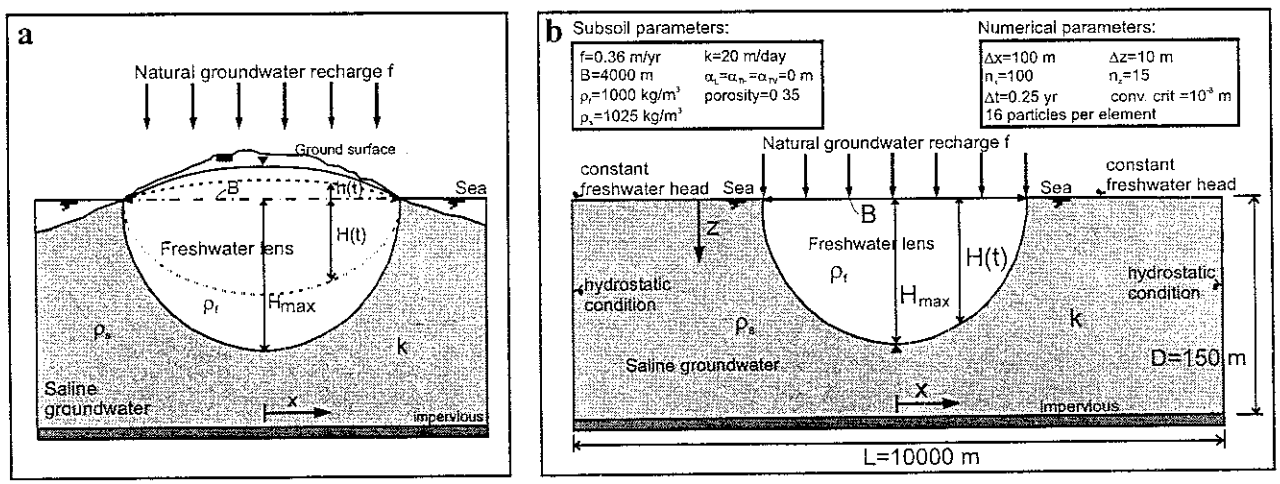

Figure 2. a. The sharp interface at an elongated island; b. Schematic representation of the problem.

The governing equations for this situation are:

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

Darcy: $$q = -k(H + h_f)\frac{\partial h_f}{\partial x}$$ (17)

[11] The Rayleigh number Ra is equal to: $Ra = \rho\alpha_f\kappa g L\Delta T/\mu\lambda$ where ρ = density of groundwater (kg m^{-3}); α_f = coefficient of thermal expansion (°C^{-1}); κ = permeability (m^2); g = gravity (m s^{-2}); L = thickness of the layer; ΔT = temperature difference between top and bottom layer (°C); μ = dynamic viscosity (kg m^{-1} s^{-1}); λ = thermal diffusivity (m^2 s^{-1}) = $\kappa_e/\rho c$ where κ_e = effective thermal conductivity (J m^{-1} s^{-1} °C^{-1}) and ρc = effective heat capacity (J m^{-3} °C^{-1})

Continuity: $$\frac{\partial q}{\partial x} = f - n\frac{\partial H}{\partial t} - n\frac{\partial h_f}{\partial t} \quad (18)$$

Note that in eq. (18) two transient terms are considered. Combination of these three equations gives:

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

This is not a linear differential equation. Hence, the equation cannot be solved analytically. However, an approximate solution is possible if is assumed that at each moment the shape of the lens is in conformation with the shape of the lens in the steady-state situation ($t\rightarrow\infty$). If so, the only difference is a time-dependent factor F(t). This results in eq. (20):

$$H(x,t) = F(t)\sqrt{\frac{f(0.25\,B^2 - x^2)}{k\alpha(1+\alpha)}} \quad (20)$$

$$\text{for } t = \infty: \quad F(t) = 1 \quad (21)$$

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

Eq. (20) is combined with eq. (19) to find the best solution, after which the differential equation is integrated from x = 0 to x = 0.5B. 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):

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

where: $$\tau = \frac{\pi n B}{8}\sqrt{\frac{(1+\alpha)}{kf\alpha}} \quad (24)$$

The factor τ is a time constant (unit T) which contains the characteristics of the geometry. For instance, for $t = 3\tau$, $\tanh(t/\tau) = 0.995 \approx 1$. This implies that at $t = 3\tau$, the shape of the fresh-water lens has nearly reached the steady-state situation. BOEKELMAN also derived formulas for the specific discharge q and the growth of the fresh-water lens. In addition, a similar derivation is given for the axial-symmetric situation (BOEKELMAN, 1998).

Based on the thickness of the fresh-water lens H, the volume of the lens can be determined:

$$V(t) = f\,B\,\tau\tanh(t/\tau) \quad (25)$$

The steady-state volume of the fresh-water lens (at $t\rightarrow\infty$) is equal to:

$$V_\infty = f\,B\,\tau = \frac{\pi n B^2}{8}\sqrt{\frac{f(1+\alpha)}{k\alpha}} \quad (26)$$

This formula obviously corresponds to the straight formula based on the form of the lens which is an ellipse: $V = \pi/4\ n\ (1+\alpha)\ H_{max}\ B$, where H_{max} = maximum depth of the fresh-water lens (m). The following parameter set is assumed in this case (fig. 2b): $\alpha = 0.025$, B = 4000 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, the time constant τ equals 73 days or 68.6 years. For the numerical computations the following parameters are applied: 16 particles per element and the convergence criterion for the groundwater-flow equation (fresh-water head) is equal to 10^{-8} metre. The total simulation time is 400 years. Two sets of discretization are considered: a) 100 by 15 elements: Δx = 100 m by Δz = 10 m, Δt = 0.25 yr; and b) 200 by 30 elements: Δx = 50 m by Δz = 5 m, Δt = 0.125 yr (decreased to obey the Courant condition). At the initial situation, the aquifer contains only saline groundwater. Figure 3 gives the evolution of the fresh-water lens at six moments in time. As can be seen, the numerical result corresponds with the analytical solution. In addition, numerical dispersion causes brackish elements. In figure 4, the increase in volume of the fresh-water lens can be seen. Note that in this comparison, the volume of the fresh-water lens derived by the phreatic part h_f is not taken into account. As such, the volume derived by the analytical solution must be multiplied by $1/(1+\alpha)$:

$$V(t) = \frac{f\,B\,\tau\tanh(t/\tau)}{1+\alpha} = 96.4\ 10^3\ \tanh(t/\tau)\ m^3/m' \quad (27)$$

As can be seen, the numerical results approach the analytical solution, though they do not really exactly match each other. This is caused by various reasons. First of all, the analytical solution suggests a one-dimensional aquifer where vertical groundwater flow is neglected, whereas MOCDENS3D simulates a two-dimensional situation with vertical groundwater velocities. This implies that in the numerical computations the outflow of fresh groundwater, equal to 0.5Bf at each side, has to exit the aquifer at x = 0.5B with huge vertical velocities. This problem of the outflow of fresh groundwater is not considered in the analytical situation. GLOVER (1959) suggested to apply a so-called outflow

width equal to 0 25Bf/αk Secondly, elements with brackish groundwater are created because of numerical dispersion of the computer code. As such, the number of elements with strictly fresh groundwater decreases, whereas the number of elements with brackish groundwater increases. As a consequence, groundwater near the interface is flowing in a different way than it does in the analytical situation. Finally, it should be noted that smaller elements increase the match, especially near the steady-state situation (compare 200*30 with 100*15 elements)

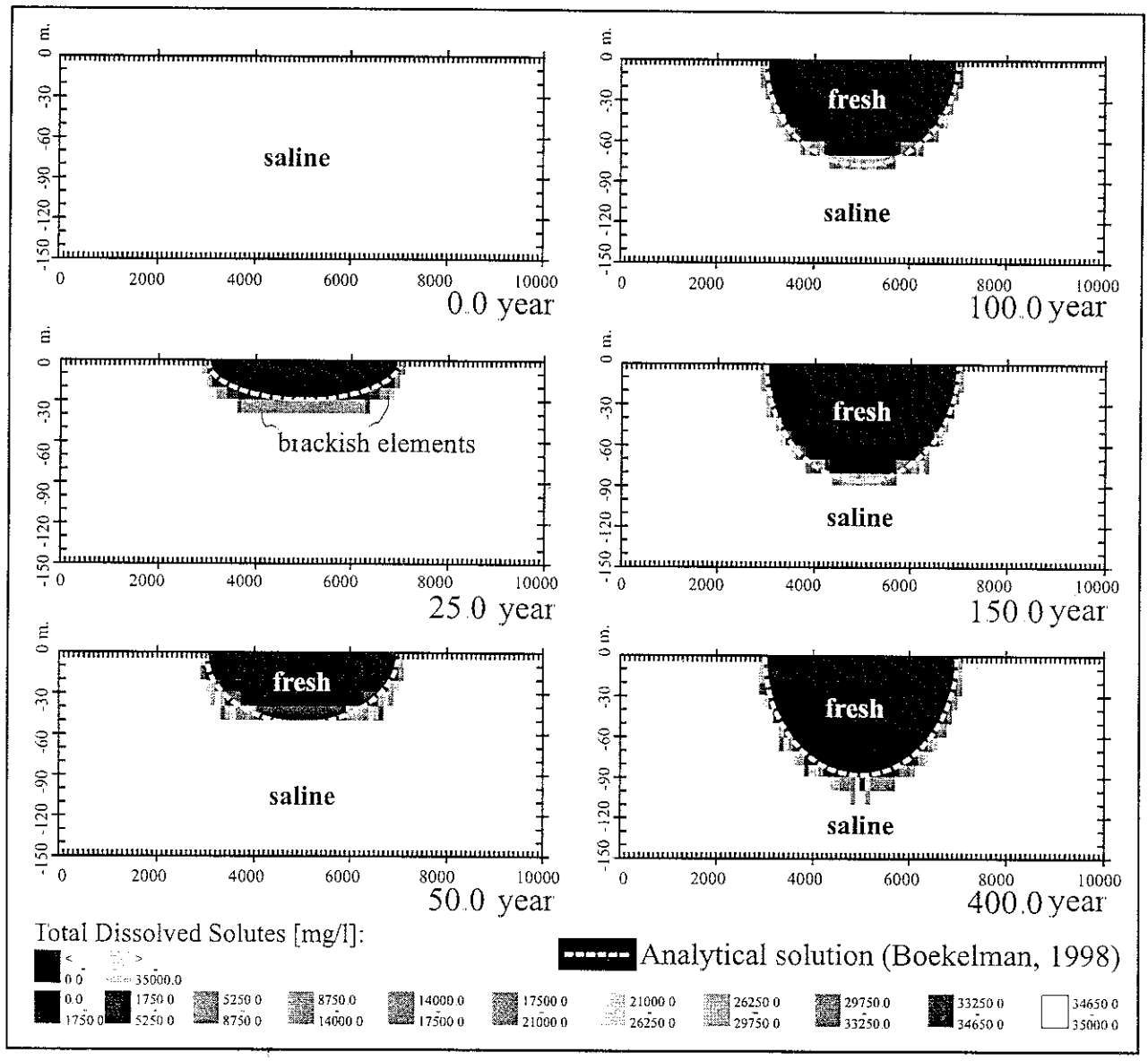

Figure 3. Evolution of the fresh-water lens: transient sharp interface between fresh and saline groundwater for the case with 100*15 elements.

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.

FUTURE DEVELOPMENTS

Recent developments in the groundwater-flow module MODFLOW are impressive. For instance, already quite a few pre- and post-processors are available (e.g. Visual MODFLOW, PMWIN, Argus ONE, GMS and Groundwater Vistas). In addition, a large number of packages and modules, besides MOC3D and MT3D96, circulate, which are compatible with MODFLOW and which can simulate to groundwater related processes, such as MODFLOWT (solute transport), RT3D and BIOMOD 3D (multicomponent transport), COMPACTION (compaction of sediments) and MODUFLOW (coupling MODFLOW and DUFLOW). Combination of MODFLOW and these packages and modules will be able to model complex problems in the (near) future.

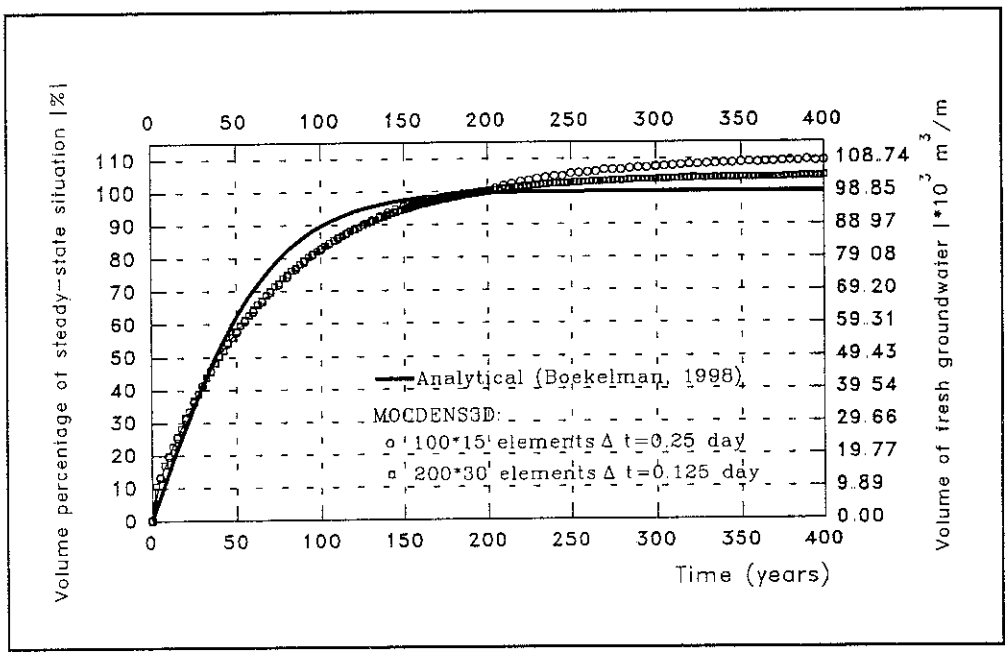

Figure 4. Evolution of the volume of the fresh-water lens. The volume is determined by the decrease in solute mass in the total aquifer system: fresh groundwater has a (suggested) concentration equal to 0 TDS mg/l whereas for saline groundwater c = 35000 TDS mg/l.

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COMPUTER ANIMATION OF THE EVOLUTION OF THE FRESH-WATER LENS

It is possible to download animations of the evolution of the fresh-water lens 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.

LIST OF SYMBOLS

B = width of the sand-dune area [L]
$C_{i\,j\,k}$ = 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}]
$CV_{i\,j\,k-1/2}$ = 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 fresh-water lens [L]
H_{max} = maximum depth of the fresh-water lens at x=0 metre [L]
h_f = fresh-water head [L]
$KV_{i\,j\,k-1/2}$ = MODFLOW term: vertical hydraulic conductivity between the elements i,j k-1and 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}]
$RHS_{i\,j\,k}$ = term in the basic equation of MODFLOW for element i,j,k, consisting of terms independent to the fresh-water 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_f = retardation factor [-]
q_z = vertical Darcian velocity (or vertical specific discharge) [L T^{-1}]
v = effective velocity [L T^{-1}]
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, resp horizontal and vertical [L]
β = coefficient of compositional expansion: e g 7 14≅10^{-7} l/mg TDS [L^3 M^{-1}]
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]
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]

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