

Variable density groundwater flow modelling with MODFLOW

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Variable density flow of groundwater can be computed by a general purpose groundwater model such as the block-centred finite-difference model MODFLOW. Density effects are accounted for by source terms that can be computed in advance. After correcting the computed intercell flows for the density effect, general purpose flow line or particle transport models such as MODPATH or MT3D can be used to generate streamlines and particle transport for the variable density situation.

Others, (Maas and Emke, 1988, Strack, 1995) have been successful in modelling regional variable density flow by means of single density models. Contrary to their work, fresh water heads are now used instead of pressures. This has many advantages in every day hydrologic practice. Further, fresh-water heads are considered easier to understand and applied in a finite difference model such as MODFLOW than the discharge potential developed by Strack for his analytical model MVAEM (1995).

Basics

In Darcy's law for volumetric three-dimensional groundwater flow under variable density conditions the flux, v [L/t], is expressed in terms of pressure, p [F/L²], the intrinsic permeability κ [L²], the fluid viscosity μ [Ft/L²] and the specific fluid weight γ [F/L³], the latter being the negative z -derivative of the hydrostatic pressure Γ [F/L²]:

$$v_x = -\frac{\kappa_x}{\mu} \frac{\partial p}{\partial x}; \quad v_y = -\frac{\kappa_y}{\mu} \frac{\partial p}{\partial y}; \quad v_z = -\frac{\kappa_z}{\mu} \left(\frac{\partial p}{\partial z} + \gamma \right) = -\frac{\kappa_z}{\mu} \left(\frac{\partial (p - \Gamma)}{\partial z} \right) \quad (1)$$

Note that the vertical coordinate, z [L], is taken positive in upward direction. The hydrostatic pressure, Γ [F/L²], is defined in terms of the specific fluid weight, γ [M/L³], as follows:

$$\Gamma = \int_{z_0}^z (-\gamma) dz \quad \rightarrow \quad \gamma = -\frac{\partial \Gamma}{\partial z} \quad (2)$$

In the sequel we'll use the fresh-water head, ϕ [L] and the hydrostatic fresh-water head, G [L], rather than pressure, p , and hydrostatic pressure, Γ . By definition:

$$\phi = \frac{p}{\gamma_0} + z; \quad G = \frac{\Gamma}{\gamma_0} + z \quad (3)$$

where γ_0 [M/L³] is fixed and set conveniently equal to the specific weight of fresh water. The hydrostatic fresh-water head, G [L], is the perfect analog of the hydrostatic pressure, Γ [F/L²]. It is alternatively and often conveniently defined directly in terms of γ as:

$$G = \frac{\Gamma}{\gamma_0} + z = -\int_0^z \frac{\gamma}{\gamma_0} dz + z = -\int_0^z \left(\frac{\gamma}{\gamma_0} - 1\right) dz \quad (4)$$

Note that both the fresh-water head and the hydrostatic fresh-water head are easily understandable physical entities. The first one being the measured head if the piezometer tube were filled over its full height with water of specific weight γ_0 , the latter can be seen as the fresh-water head in case that "no water were flowing" relative to some reference level taken $z=0$ here for convenience. Since the density distribution is considered given, the hydrostatic fresh-water head can be computed in advance.

Filling in $p = \gamma_0(\phi - z)$ in the Darcy equations above, we obtain the Darcy equations in terms of fresh water heads:

$$v_x = -k_x \frac{\partial \phi}{\partial x}; \quad v_y = -k_y \frac{\partial \phi}{\partial y}; \quad v_z = -k_z \left(\frac{\partial \phi}{\partial z} + \frac{\gamma}{\gamma_0} - 1 \right) = -k_z \left(\frac{\partial(\phi - G)}{\partial z} \right) \quad (5)$$

in which the usual permeabilities, k [L/t], replace the coefficients $\kappa\gamma_0/\mu$. Both forms of Darcy's equations are perfectly analogous. Note that the combined term $\Phi = \phi - G$ is called the environmental head after De Wiest (1969), because it produces the vertical flow in density situations if differentiated with respect to z .

Horizontal flow in MODFLOW cells

In density flow computations the head and the flows may be strongly dependent on the density distribution of the fluid. The water may flow to the right in the top of an aquifer and at the same time to the left at its bottom. Hence we have to consider the gradient variation even within model cells. The block centred finite difference model only computes heads at the centre of each cell. So we must consider the head variation relative to the value at the cell centre.

We obtain the head at some height z , above or below the cell centre, $z=M$, by integrating the vertical head gradient given by Darcy (eq. 5) accordingly:

$$\frac{\partial \phi}{\partial z} = -\frac{v_z}{k_z} + \frac{\partial G}{\partial z} \rightarrow \phi_z = \phi_M + G_z - G_M - \int_M^z \frac{v_z}{k_z} dz \quad (6)$$

Within a model cell k_z is considered constant, while v_z is considered to vary only with z and so it vanishes when the head is differentiated with respect to x or y in order to compute the horizontal flow components at elevation z . Hence the horizontal x -component of the groundwater flow at elevation z is expressed in the head at the cell centre and the hydrostatic fresh-water head:

$$v_x = -k_x \frac{\partial \phi_M}{\partial x} - k_x \frac{\partial(G_z - G_M)}{\partial x} \quad (7)$$

In order to obtain the horizontal flow, Q_x [L³/t], in x -direction through a model cell of given height Δz [L] (fig. 1), we integrate v_x over the full height of the cell and multiply by the cell width Δy [L]:

$$Q_x = \Delta y \int_{z_B}^{z_T} v_x(z) dz = -k_x \Delta y \Delta z \left[\frac{\partial \phi_M}{\partial x} + \frac{\partial (\bar{G} - G_M)}{\partial x} \right] \quad (8)$$

Where the \bar{G} denotes the average hydrostatic head taken at the x -location over the full height of the cell. Hence $\bar{G} - G_M$ represents the deviation of the average hydrostatic fresh-water head over the height of the model cell from its value at half the height of the cell. This term is zero if the density is constant over the cell height, because in that case the hydrostatic fresh-water head is a linear function of z at any location.

Between the midpoints of two adjacent model cells A and C (fig. 1) Q_x is considered constant, $Q_{AC} = Q_x$, only to jump at the cell centers. So, to express the horizontal flow in the heads in the cell centers, we integrate the head gradients between these two points A and C, passing through the points BL and BR at the left- and right-hand side of the cell wall, B, between the two cells (fig. 2). Note that, while Δz may vary from cell to cell, Δx and Δy are constant per column and row:

$$Q_{AC} \int_A^C \frac{1}{k_x \Delta y \Delta z} dx = - \int_A^C \frac{\partial \phi_M}{\partial x} dx - \int_A^C \frac{\partial (\bar{G} - G_M)}{\partial x} dx \quad (9)$$

This yields:

$$Q_{AC} = C_{AC} [(\phi_A - \phi_C) - (\phi_{BL} - \phi_{BR}) + (\bar{G}_A - G_A) - (\bar{G}_{BL} - G_{BL}) + (\bar{G}_{BR} - G_{BR}) - (\bar{G}_C - G_C)] \quad (10)$$

Where C_{AC} [L²/t] is the MODFLOW conductance (McDonald and Harbaugh, 1988):

$$C_{AC} = \Delta y / \left[\frac{\Delta x_A / 2}{k_A \Delta z_A} + \frac{\Delta x_C / 2}{k_C \Delta z_C} \right] \quad (11)$$

The fresh-water head difference $\phi_{BL} - \phi_{BR}$ has to be evaluated with care, because the hydrostatic fresh water head doesn't have to be continuous across the cell wall. Neglecting the resistance against vertical flow in this cell boundary plane we can express this term in terms of precalculated hydrostatic fresh-water heads (fig. 2):

$$\phi_{BR} - \phi_{BL} = (G_{BR} - G_{MR}) - (G_{BL} - G_{ML}) = \Delta G_{BR} - \Delta G_{BL} \quad (12)$$

So finally we have, in a most general sense, the following expression for the horizontal volumetric flow between adjacent cells A and C, as shown in fig. 2:

$$Q_{AC} = C_{AC} (\phi_A - \phi_C) + C_{AC} [(\bar{G}_A - G_A) - (\bar{G}_C - G_C) - (\bar{G}_{BL} - G_{BL}) + (\bar{G}_{BR} - G_{BR}) - (\Delta G_{BL} - \Delta G_{BR})] \quad (13)$$

The first term on the right hand side represents the effect of the fresh water head on the flow, the second part

represents the effect of density variations. The latter is a fixed value, since the all hydrostatic fresh-water heads are assumed to be given. If brought to the left side of the equation it represents a fixed source term to be added to other fixed source terms before running the model. If left at the right hand side of the equation, as in the above form, it represents a correction on the horizontal flow computed by the model, in order to obtain the true volumetric flow between the cells A and C. Clearly, the same equation holds true in both the x and y directions.

PRACTICAL SIMPLIFICATION: Often, one will be tempted to simplify the model by assuming either a single density value in each cell or a density distribution that is independent of x,y within each cell, for instance by assuming a cell-wise horizontal interface between fresh and salt water. In such cases we have:

$$(\overline{G}_A - G_A) = (\overline{G}_{BL} - G_{BL}) \quad \text{and} \quad (\overline{G}_C - G_C) = (\overline{G}_{BR} - G_{BR}) \quad (14)$$

so that then all terms that express the difference between de height-averaged hydrostatic head and their value at half the cell's height vanish. This leaves us with:

$$Q_{AC} = C_{AC} (\phi_A - \phi_C) - C_{AC} (\Delta G_{BL} - \Delta G_{BR}) \quad (15)$$

The right term can be elaborated explicitly in the special case of a single density per cell or per layer as was used by Maas and Emke (1988). We can, however, in all cases just as well precalculate G and use that.

If we assume within each cell a density that is independent of x,y and at the same time adopt a regular model mesh, such that the tops and bottoms of the cells in a model layer all match, then the horizontal flow between two adjacent cells simplifies to the equation for the fresh-water model (refer to eq. 12):

$$Q_x = C_{AC} (\phi_A - \phi_C) \quad (16)$$

Use of one density per layer can often be achieved by splitting model layers in sublayers at planes separating zones of constant but distinct density, such as the interface between fresh and salt water (Maas and Emke, 1988). Use of a single density per cell is often acceptable with small salinity gradients. We tend to use cell-wise horizontal interface or simply use the given full equation for horizontal flow. In any case, it should be noted that all terms comprising the specific fluid weight, γ , and hence the hydrostatic fresh-water head, G, can be computed in advance.

Vertical flow

To discretize the equation for vertical flow, we integrate the head gradient of the vertical flow equation (eq. 5) between the centres of two cells situated above one another (fig. 3).

$$\int_{z_A}^{z_B} \frac{v_z}{k_z} dz = - \int_{z_A}^{z_B} \frac{\partial \Phi}{\partial z} dz = - \int_{z_A}^{z_B} \frac{\partial (\phi - G)}{\partial z} dz \quad (17)$$

If we consider the three different permeabilities between point A and B as shown in fig. 3, we obtain:

$$v_z \left(\frac{\Delta z_A / 2}{k_{z_A}} + \frac{D}{k_z} + \frac{\Delta z_B / 2}{k_{z_B}} \right) = (\phi_A - \phi_B) - (G_A - G_B) \quad (18)$$

or, for the total volumetric flow $Q_{AB} = \Delta x \Delta y v_z$

$$Q_{AB} = C_{AB} (\phi_A - \phi_B) - C_{AB} (G_A - G_B) \quad (19)$$

in which C_{AB} [L²/t] is the vertical MODFLOW conductance or leakance (McDonald and Harbaugh, 1988):

$$C_{AB} = \Delta x \Delta y / \left[\frac{\Delta z_A / 2}{k_{z_A}} + \frac{D}{k_z} + \frac{\Delta z_B / 2}{k_{z_B}} \right] \quad (20)$$

Like the horizontal flow, the first term of the equation represents the vertical flow computed by the model, while the second term is a density source term, if brought to the left side of this equation. So, it has to be added to the other ordinary source terms (such as wells) before running the model. The right-hand term has to be subtracted from the flows calculated by the model in order to obtain the true flow, Q_{AB} , for the variable density case. Note that the right hand term is zero in the fresh-water part of the model.

Water balance for a model cell

Providing indices N,E,S,W,T,B to indicate the cell to the North, East, South, West, Top and Bottom of the considered cell, we write down the water balance of a MODFLOW cell:

$$Q_E + Q_N + Q_W + Q_S + Q_T + Q_B + Q_G + Q = 0. \quad (21)$$

In which the index "G" stands for all indirect, that is, head dependent "general head boundaries", including rivers and drains:

$$Q_G = \sum_{j=1}^m [C_j (G_j - G_0)] \quad (22)$$

Where the index "0" denotes the considered cell and C_j is the corresponding conductance. The sum is taken over all external heads connected to the considered cell. Q is the total direct input for the cell. Note that all values are taken positive if their direction is inward, that is, when they raise the head in the cell that is being considered.

Because all hydrostatic fresh-water head terms are considered to be known in advance, they can be put to the right hand side of the above cell balance (eq. 21), together with the direct inputs (wells). Filling in the formulas for horizontal and vertical flow (eqs. 13 and 17), we obtain in the most general case:

$$\begin{aligned}
& C_E \phi_E + C_N \phi_N + C_W \phi_W + C_S \phi_S + C_T \phi_T + C_B \phi_B + \sum C_G \phi_G \\
& - (C_E + C_N + C_W + C_S + C_T + C_B + \sum C_G) \phi_0 = \\
& \quad - C_E ((\overline{G}_E - G_E) - (\overline{G}_0 - G_0) - (\overline{G}_{EE} - G_{EE}) + (\overline{G}_{E0} - G_{E0}) - (\Delta G_{EE} - \Delta G_{E0})) \\
& \quad - C_N ((\overline{G}_N - G_N) - (\overline{G}_0 - G_0) - (\overline{G}_{NN} - G_{NN}) + (\overline{G}_{N0} - G_{N0}) - (\Delta G_{NN} - \Delta G_{N0})) \\
& \quad - C_W ((\overline{G}_W - G_W) - (\overline{G}_0 - G_0) - (\overline{G}_{WW} - G_{WW}) - (\overline{G}_{W0} - G_{W0}) - (\Delta G_{WW} - \Delta G_{W0})) \\
& \quad - C_S ((\overline{G}_S - G_S) - (\overline{G}_0 - G_0) - (\overline{G}_{SS} - G_{SS}) - (\overline{G}_{S0} - G_{S0}) - (\Delta G_{SS} - \Delta G_{S0})) \\
& \quad + C_T (G_T - G_0) \\
& \quad + C_B (G_B - G_0) \\
& \quad + \sum C_G (G_G - G_0) \\
& \quad - Q
\end{aligned} \tag{23}$$

The index "0" to denotes the considered cell. The index "EE" denotes the East-side of the boundary plane between the considered cell and its eastern neighbour; the index "E0" denotes the boundary plane between the eastern cell and the considered cell at the side of the considered cell. "E" is replaced accordingly by "N", "W" and "S".

The left hand side of eq. 23 represents the internal structure of the finite difference model, i.e. MODFLOW, and the right-hand side represents its source terms. So we can obtain the fresh-water head under variable density conditions by using the right-hand side as the source term and running our ordinary ground-water model.

Boundary conditions

Direct boundary flows from or to wells are unchanged in the variable density situation. Given heads must be specified in terms of fresh-water heads. Boundaries with horizontal flow require v_z to be zero and so the head must equal the hydrostatic fresh-water head but for a constant:

$$\frac{\partial \phi}{\partial z} = \frac{\partial G}{\partial z} \rightarrow \phi = G + Constant \tag{24}$$

Horizontal boundaries that are closed also have a zero vertical flow component. This is achieved here by a using a boundary flow equal to $-k_z \partial G / \partial z$

$$v_z = -k_z \frac{\partial \Phi}{\partial z} = -k_z \frac{\partial (\phi - G)}{\partial z} = 0 \rightarrow -k_z \frac{\partial \phi}{\partial z} = -k_z \frac{\partial G}{\partial z} \tag{25}$$

Hence, the model must be given the right-hand term as a source term at this boundary in order for it to be impermeable. This, however, is automatically guaranteed by proper computation of the vertical density source terms.

Use of the equations

The density source terms are composed of contributions from all cell faces (E, N, W, S, T, B) and different kind of general head boundaries. These individual components are computed first and put in a budget file to be used later to correct the intercell flows before applying MODPATH or MT3D. Then the terms for each cell are summed and merged into the well input file. Finally, MODFLOW is run to obtain the fresh-water heads for the variable density case.

In many cases this is all we need, since fresh-water heads are exactly what we need in the fresh-water part

of the model. They are also correct for the saline part, but as is generally the case with density flow, interpretation in terms of flow is somewhat more complicated.

Also, the flows in the fresh water part of the model are immediately usable. Hence transport models will produce the right results in this part of the model right away. But the intercell flows in the saline part of the model have to be corrected before MODPATH and MT3D yield the correct particle transport. All we have to do before using MODPATH or MT3D is to subtract the corresponding density source term components from the computed intercell flows residing in the budget file freshly computed by MODFLOW.

Rapid modelling of variable density flow

There are several tricks to have MODFLOW itself compute and output its conductances and density source terms by using proper initial heads and run MODFLOW with zero iterations. Limited space allows only to indicate this here. For instance, if the density can be simplified as independent on x,y within a model cell, and we use a regular model mesh, such that the tops and bottoms of the cells in a layer match exactly, the former water balance equation reduces to:

$$\begin{aligned}
 &C_E\phi_E + C_N\phi_N + C_W\phi_W + C_S\phi_S + C_T\phi_T + C_B\phi_B + \sum C_G\phi_{G_C} \\
 &- (C_E + C_N + C_W + C_S + C_T + C_B + \sum C_G)\phi_0 = \\
 &+ C_T(G_T - G_0) + C_B(G_B - G_0) + \sum C_G(G_G - G_0) - Q
 \end{aligned} \tag{26}$$

This allows very easy computation of variable density flow, since the right-hand source terms can now be readily computed by the model itself. This is achieved by first setting $Q=0$, then making $C_E=C_N=C_W=C_S=0$ and finally running MODFLOW with zero iterations, with the initial heads and external heads (rivers and so on) the precomputed hydrostatic fresh-water head, G . This makes the left-hand side of the above equation equivalent to the right-hand side. Thus the model itself will produce the density-source terms specified at the right-hand side of the above equation in MODFLOW's budget file. After totalling them per cell and adding them to the other source terms (wells, i.e. the given Q -values) the model is run a second time to compute the wanted fresh-water heads throughout the model for the variable density situation. The new intercell flows are stored in MODFLOW's the budget file. They have to be corrected before using MODPATH or MT3D by subtracting the source density terms stored in the first budget file.

Hence solving a variable density groundwater problem in the case of a regular mesh and a single density per model cell is reduced to running the model twice. If the mesh is not regular, but the density is constant per layer, the model has to be run three times. (This may not only be true for a regular and easily understood finite difference model such as MODFLOW, but just as well for any finite element model, which we leave to be proved by others.). In more general cases the easiest way will be to compute these terms by a separate program. Note that the conductances can be obtained from MODFLOW using initial heads such that the head difference between adjacent cells in x, y and z direction always equals unity.

Example

Simple examples, concerning flow in a vertical cut, have already been given by Olsthoorn (1996). So here a more complicated example is presented to demonstrate the potential of the method. Here we show the applications applied on the MODFLOW model of the Amsterdam dune area (Olsthoorn e.a. 1993, Kamps and Olsthoorn, 1996) that contains 13 layers, i.e. 7 aquifers and 6 aquitards.

The cells of a layer do not match in height, but we assume, just for this example, that the density within a cell only depends on z, (such as a piecewise horizontal interface or a single density per cell). Hence, all horizontal density terms containing an overlined (i.e. height averaged) hydrostatic fresh-water head vanish from the general water balance equation. For now we assume a sharp interface crossing a great number of cells. This sharp interface allows easy precomputation of the hydrostatic fresh water head, G , everywhere in the model. It equals the depth below the interface times $(\gamma/\gamma_0 - 1)$.

Figure 4 shows a west-east cross section running from the North Sea in the west 4.4 km land inward, showing the computed fresh water heads and the wells. (The dark skyline is the dry part of the phreatic top aquifer). Above the interface the fresh-water head isolines directly show the flow situation; below it, the effect of density on the fresh-water head is manifest. There the flowlines will not be perpendicular to the isolines.

Figure 5 shows the flow situation and the layers. The arrows have been computed by MODPATH, they are in fact small pathlines of 100 days duration starting at equidistant locations with an arrow head placed at 100 days (i.e. at the end of the path). The result is a clear flow picture, clarifying among others the predominant vertical flow through the aquitards. Before running MODPATH the intercell flows in the budget file have been corrected by the density flow source terms. Clearly, below the interface the flow is no longer perpendicular to the fresh-water heads.

Of course, cells that are intersected by the interface cannot within MODFLOW reveal the details of the density flow within them. However the total flow over each cell boundary is always correct. Still, more detail can be obtained by splitting layers of interest or by applying the horizontal gradient for height z above the centre of the cell using the details of the density distribution, as given in equation 7.

We use Matlab (see <http://www.mathworks.com> on the world wide web for details) to compute the hydrostatic fresh water heads and the density source terms directly from the data. Matlab is efficient in handling matrices and so to compute coefficients from a block-shaped model such as MODFLOW. Matlab is also used to alter the budget file by subtracting the density source terms from it before running MODPATH. (You may E-mail me for the Matlab mfiles). Visualization is done conveniently in Visual MODFLOW (see Scientific Software Catalogue) from which the figs. 4 and 5 were produced as well. Using Matlab our basic data are immediately shaped into Visual MODFLOW files. These are somewhat easier to handle than those of MODFLOW, while an import phase is omitted. Visual MODFLOW produces the needed MODFLOW and MODPATH files, launches the latter models and reads their results back in for visualization.

It is concluded that the method is practical and works well in complex three-dimensional situations. It could be readily implemented in a MODFLOW-module if someone were willing to invest some time to realise it. The next step to be developed would be the movement of the density along with the water flows.

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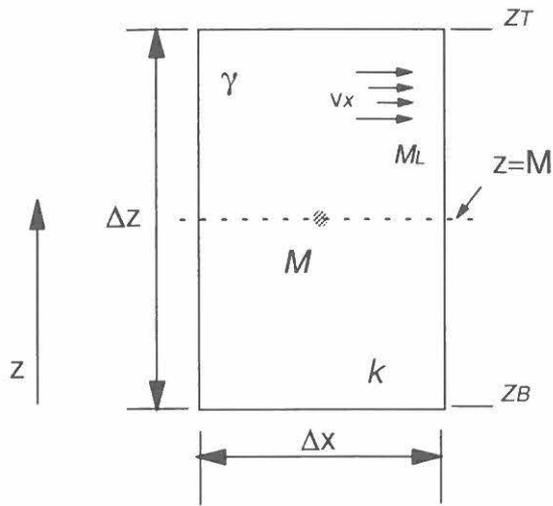


Fig. 1: Single MODFLOW cell, in vertical cross section

Fig. 2: Horizontal flow between two MODFLOW cells of different height.

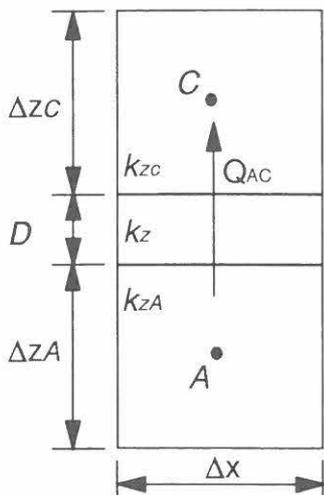
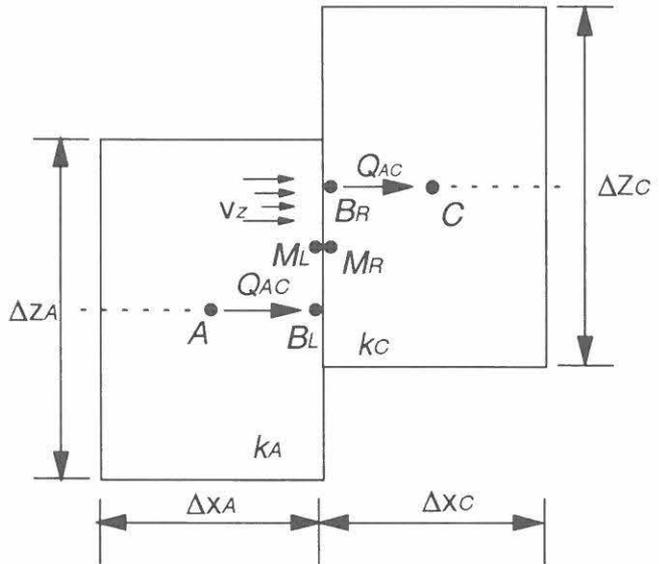


Fig. 3: Vertical flow between two overlaying MODFLOW cells, separated by an intermediate layer (aquitard).

Fig. 4: (Top next page) Cross section from the North Sea in the West through Amsterdam Dune Area, showing aquifers, aquitards and isolines of the computed fresh-water heads (m + mean sea level). The "Sky line" represents unsaturated dunes. Sharp fresh-saline water interface as indicated. Note the effect on the isolines.

Fig. 5: (Bottom next page) Same cross section as fig. 4, showing path lines of 100 day lengths with arrow heads at their ends. These pathlines have been computed by MODPATH, after first subtracting the density effect (terms containing "G" in eq. 10 and 19) from the intercell flows computed by MODFLOW. Note that the pathlines are not perpendicular to the fresh-water head isolines in the saline part of the groundwater system.

